제 21 회 유기화학분과회 하계워크샵

■ 일시: 2021 년 6 월 28~29 일

■ 장소: 페어필드바이메리어트 송도 비치, 부산

■ 주관: 대한화학회

■ 주최: 유기화학분과회

| 공식후원사 | TCI · SEJIN CI

Korean Chemical Society
Division of Organic Chemistry

유기화학분과회 하계워크샵 참석 회원님께,

반갑습니다 !

작년 내내 만남을 갖지 못해 아쉬움이 커 올해 이렇게 용기를 내어 유기분과회 하계워크샵을 부산 송도에서 대면으로(젊은 유기화학자상 시상식 및 수상 강연은 대면/비대면 혼용) 개최하게 되었습니다.

제 21 회 유기화학분과회 하계워크샵에 참석하신 모든 회원님을 환영합니다. 코로나 상황 때문에 지난주 까지도 계획처럼 진행할 수 있을지 조마조마하였습니다. 참석 인원이 100 명을 넘지 않으며, 방역수칙을 철저히 지키는 전제로 진행하기에 예년같이 즐거운 시간을 함께 갖지 못하게 되어 죄송스럽고 아쉽게 생각합니다. 저희에게 큰 추억을 남겨주던 학생들과의 동반 참석은 내년을 기약하게 되었습니다.

2019 년 이후 처음 가지는 모임이어서 이번에는 가능한 많은 분께 짧게나마 발표 기회를 드리고자 기획하였습니다. 코로나 상황으로 인해 부득이 2 개의 세션으로 나누어 발표를 진행하고자 합니다. 41 명의 회원께서 발표하시는 관계로 충분한 질의/응답 시간을 가질 수 없지만 대신 배부되는 피드백 용지에 코멘트 등을 적어 각 발표자분께 전달해 조금이라도 알찬 도움을 드리고자 합니다.

올해 젊은 유기화학자상 수상자로 선정되신 충북대학교 김민 교수님께 큰 축하를 드립니다. 특히 충북대학교 김민 교수님의 시상식 및 수상강연은 온라인을 통해 동시 송출할 것인바 회원님 및 회원님 소속 연구실 대학원생들의 많은 참여를 부탁드립니다.

본 하계 워크샵을 준비하고 진행하는데 재정적으로 후원을 해주신 여러 회사와 회원님들께 깊은 감사를 드립니다 (리스트가 아래에 있습니다).

다시 한번 격하게 환영하며(!) 이번 하계 워크샵이 모든 분께 유익한 학술교류의 장이 되며 또한 짧지만 즐거운 시간으로 기억되기를 기원합니다.

2021 년 6 월 28 일

유기화학분과회 운영진
(장석복, 이선우, 강은주, 주정민, 천철홍, 한순규, 곽재성, 이민희)

구분	후원 기관	
학교	서울대학교 이철범 교수 연구실	서울대학교 유기화학실험실 Organic Chemistry Laboratory
회사	㈜세진씨아이 (공식후원)	TCI · SEJIN CI
회사	대정화금	DAEJUNG CHEMICALS & METALS
회사	BK 인스트루먼트(BKI)	BK Instruments Inc.
회사	보로노이바이오 / B2SBio	
회사	브루커코리아㈜	BRUKER
회사	사이플러스	사이플러스 Science plus
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회사	이우과학교역	(주) 이 우 과 학 교 역 IWOO Scientific Corporation
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송충의(성균관대)	신광민(성균관대)	신승훈(한양대)	우상국(울산대)
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홍순혁(KAIST)	홍승우(KAIST)	NIMSE SATISH BALASAHEB(한림대)	

장소: 페어필드바이메리어트 부산 송도 비치

(주소: 부산 서구 송도해변로 113, 전화: 051-260-0000)

※ 오시는 방법: 부산역에서 택시 20 분, 또는 버스 17, 26, 61 번 이용

※ 2021 년 6 월 28 일(월) ※

■ 제 1 강연장(2 층)

	줌 링크: https://zoom.us/j/4217755535	
10:30~10:35	개회사: 장석복 (KAIST) (온/오프라인)	진행: 이선우
10:35~10:40	**젊은 유기화학자상 시상식 (온/오프라인)**	진행: 강은주
10:40~11:10	**젊은 유기화학자상 수상강연 (온/오프라인)** **김민 (충북대학교)** **Development of MOF-based Catalysts with Organic Chemistry**	

■ 제 1 강연장(2 층)

Session I	발표자	좌장: 강은주	발표 제목
13:00~13:10	기정민	UNIST	Chemical Tools to Explore the "Hidden" Protein Phosphorylations
13:10~13:20	정병혁	DGIST	Stereoselective Synthesis of (*E*)- and (*Z*)-α-Silyl-α,β-unsaturated Amides with DIBAL-H and Isocyanates
13:20~13:30	이충환	가천대	Synthetic Studies of Natural Products: Curcusones and Mechanistic Elucidation of an Unexpected Rearrangement
13:30~13:40	임창수	아주대	New Photodynamic Therapy Methods and Applications Selective for Two-Photon Excitation
13:40~13:50	이효준	군산대	Acyl Fluoride Generation Promoted by Hypervalent Iodine(III) Reagents: Effective Method for Hindered Amide-Bond Formation
13:50~14:00	김범진	울산대	Enzyme-Catalyzed Self-Assembly of Peptide for Selective Inhibition of Cancer Cells
14:00~14:10	이상기	이화여대	Cooperative Pd(0)/Rh(II) Dual Catalysis for the Synthesis of Heterocyclic Compounds
14:10~14:35	Break Time		

Session II	발표자	좌장: 김민	발표 제목
14:35~14:45	장영태	POSTECH	New Approach for Live Cell Distinction through Lipid (LOLD)
14:45~14:55	김기태	충북대	Peptide Nucleic Acid-based Hybridization Chain Reaction (HCR) for Imaging of Cellular Targets
14:55~15:05	우상국	울산대	Visible-Light Photoredox-Catalyzed Selective Transformation of Oxaziridines into Nitrones and Amides
15:05~15:15	손종우	동아대	Manganese-Catalyzed Late-Stage C–H Diversification of Peptides: Modular Synthesis of Fluorogenic Probes
15:15~15:25	정시원	목포대	Utilization of the N-Silyl Enamine Intermediate from N-Heteroarene: Synthesis of Cyclic Amidines and Bicyclic Pyrazolidine Derivatives
15:25~15:35	김재현	강원대	α-C-H Bond Functionalization of Unprotected Cyclic Amines via Transient Imines
15:35~15:45	홍성유	UNIST	Directed and Non-Directed Annulative π-Extension Reactions
15:45~16:30	Group Photo Session & Break Time		
Session III	**발표자**	**좌장: 김학중**	**발표 제목**
16:30~16:40	류도현	성균관대	Highly Enantioselective Synthesis of Trisubstituted Epoxides: Catalytic Asymmetric Darzens-type Epoxidation of Diazoesters
16:40~16:50	김인수	성균관대	P- and S-Ylides for C–H Functionalization of N-Heterocycles
16:50~17:00	장혜영	아주대	Synthesis of Triscarbene-Modified Iridium Catalysts and Their Application to β-Alkylation of Alcohols
17:00~17:10	조우경	충남대	Synthesis of Zwitterionic L-DOPA and its Applications to Virus Immunoassay/Medical Implant
17:10~17:20	임희남	영남대	DAST-mediated C–C Bond Cleavage of Activated Carbonyl Compounds
17:20~17:30	강경태	경희대	Chemistry of Amyloids and Catechols
17:30~17:40	홍석원	GIST	Development of Chiral Pyridine-Dihydroisoquinoline Ligands
17:40~	Dinner & Free Time		

■ 제 2 강연장(22 층)

Session I	발표자	좌장: 주정민	발표 제목
13:00~13:10	이준석	고려대	Photo-activation Approach to Spatio-temporal Mapping for Biomolecule Interactions in Complex Biological Environment
13:10~13:20	김현우	이화여대	Electrochemically Driven Stereoselective Approach to syn-1,2-Diol Derivatives from Vinylarenes and DMF
13:20~13:30	이원철	강원대	Synthetic Studies toward the Total Synthesis of Arenaric Acid
13:30~13:40	한지훈	안동대	Highly Sensitive and Selective Mercury Sensor Based on Mismatched Base Pairing with dioxT
13:40~13:50	서성은	아주대	Cu-Catalyzed Isocyanation of Benzylic C–H Bonds Enabling High-Throughput Synthesis of Diverse Pharmaceutically Relevant Ureas
13:50~14:00	이민재	군산대	Cyclic Bis-ammonium Salts as a New Class of Organic Ionic Plastic Crystals (OIPCs)
14:00~14:10	김병문	서울대	A Novel Approach for Tuberculosis Chemotherapy Through Disruption of Bacterial Toxin-Antitoxin Systems
14:10~14:35	Break Time		
Session II	**발표자**	**좌장: 정원진**	**발표 제목**
14:35~14:45	이용록	영남대	In(III)-Catalyzed Regioselective Syntheses of 1-Naphthaldehydes from 3-Formylchromones
14:45~14:55	강호웅	충북대	Asymmetric Oxidative Phenol Coupling to Install Axial Chiral Bonds and Its Application in Chaetoglobin A Synthesis
14:55~15:05	손정훈	충남대	Copper-Mediated Oxidative Dehydrosulfurative Carbon-Nitrogen Cross-Coupling of 3,4-Dihydropyrimidine-2-thiones with Amines
15:05~15:15	김용주	고려대	Supramolecular Chemistry for Biofunctional Materials
15:15~15:25	김도경	경희대	Functional Fluorescent Probes for Image-guided Surgery of Human Glioblastoma

15:25~15:35	신광민	성균관대	Group 10 Transition Metal (Ni, Pd)-Catalyzed Asymmetric Hydro-functionalization of Alkenes
15:35~15:45	Satish Balasaheb Nimse	한림대	An Abiotic Fluorescent Probe for the Detection and Quantification of Carcinoembryonic Antigen
15:45~16:30	Group Photo Session & Break Time		
Session III	**발표자**	**좌장: 이안나**	**발표 제목**
16:30~16:40	홍승우	KAIST	Investigation of Regioselective C–H Functionalization of Heteroarene
16:40~16:50	서지원	GIST	Interplay among Conformation, Intramolecular Hydrogen Bonds, and Chameleonicity in the Membrane Permeability and Cyclophilin A Binding of Macrocyclic Peptide Cyclosporin O Derivatives
16:50~17:00	유은정	경희대	Fascinating Construction and Restructure of N-Heterocyclic Compounds
17:00~17:10	이윤미	광운대	Cu-Catalyzed Hydroalumination of Allenes with DIBAL-H: Synthesis of α-Quaternary Carbon Centers
17:10~17:20	홍대화	부산대	Development of Versatile Initiator Films for Surface-Initiated Polymerization
17:20~17:30	송충의	성균관대	Water-Driven Biomimetic Catalytic Enantioselective Protonation
17:30~	Dinner & Free Time		

※ 2021 년 6 월 29 일(화) ※

9:00~11:00	그룹별 자유토론
11:00 ~	폐회식 및 귀가

■ 제 10 회 젊은 유기화학자상 수상자

김민

충북대 화학과 교수

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2012-현재: 충북대학교 조교수/부교수/교수

2010-2012: UC San Diego, 박사후연구원

2010: KAIST, Ph.D.

2006: KAIST, M.S.

2004: KAIST, B.S.

Positions, Services, Representative Awards

2020 – Present	Executive Director of General Affair Team in KCS
2020	Young Investigator Award by KSOS
2020	Thieme Chemistry Journals Award
2019 – Present	Department Chair, Department of Chemistry, Chungbuk National University
2018 – 2019	Committee of Organic Chemistry Division in KCS
2014	ACP Lectureship Award from Malaysia

Representative Publications

1. Kim, S.; Lee, H.-E.; Suh, J.-M.; Lim, M.; Kim. M. "Sequential Connection of Mutually Exclusive Catalytic Reactions by a Method Controlling the Presence of a MOF Catalyst: One-Pot Oxidation of Alcohols to Carboxylic Acids" *Inorg. Chem.* **2020**, *59*, 17572-17582.

2. Kim, S.; Lee, J.; Jeoung, S.; Moon, H. R.; Kim, M. "Surface Deactivated Core-Shell Metal-Organic Framework by Simple Ligand Exchange for Enhanced Size Discrimination in Aerobic Oxidation of Alcohols" *Chem. Eur. J.* **2020**, *26*, 7568-7572.

3. Han, J.; Lee, M. S.; Thallapally, P. K.; Kim, M.; Jeong, N. "Identification of Reaction Sites on Metal-Organic Framework-Based Asymmetric Catalysts for Carbonyl-Ene Reactions" *ACS Catal*. **2019**, *9*, 3969-3977.

4. Kim, S.; Kim, Y.; Jin, H.; Park. M. H.; Kim, Y.; Lee, K. M.; Kim, M. "Europium-Catalyzed Aerobic Oxidation of Alcohols to Aldehydes/Ketones and Photoluminescence Tracking" *Adv. Synth. Catal*. **2019**, *361*, 1259-1264.

5. Hahm, H.; Yoo, K.; Ha, H.; Kim, M. "Aromatic Substituent Effects on the Flexibility of Metal-Organic Frameworks" *Inorg. Chem.* **2016**, *55*, 7576-7581.

Development of MOF-based Catalysts with Organic Chemistry

Min Kim
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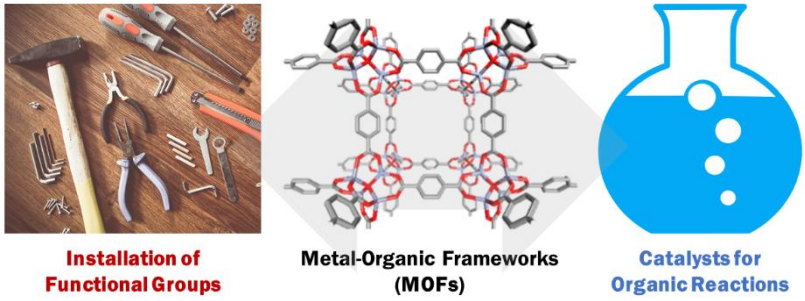
Metal-Organic Frameworks (MOFs, also called PCPs, porous coordination polymers) are 3D porous materials, which are constructed from coordination bonds between metal clusters (or ions) and multitopic ligands such as benzene-1,4-dicarboxylic acid. Due to their permanent porosity, structural diversity, and low density, various applications such as gas adsorption, molecular separation, and molecular shuttling have been deeply investigated during last two decades. In addition to sieving effect, the tunability of structure is also considered as a great advantage of MOFs. Especially, the organic ligand parts of MOFs (*i.e.*, strut of MOF framework) could be modified and functionalized with organic functional groups in relatively ease manners toward target applications.[1]
In this perspective, MOFs have also been considered a good platform for heterogeneous catalyst toward various organic reactions. The specific functionalizations with organometallic species and the dispersion of metal catalyst to porous MOF structures allowed a highly active, heterogeneous catalysts for organic transformations.[2] In addition, the positional functionalizations (*e.g.*, surface vs. core) are possible in this hybrid-heterogeneous material. Therefore, multifunctional, catalytic materials have been achieved in MOF platform with several organic chemistry techniques. In this presentation, our recent developments for selective MOF-based catalysts will be covered, especially for size-selective carbonyl-ene reactions and size-selective and chemo-selective aerobic oxidation of alcohols.[3-5]



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김 민

조교수, 부교수, 교수: 충북대학교 화학과 (2012~현재)
연구분야: Developments of metal-catalyzed organic reactions, functionalizations and catalytic applications of metal-organic frameworks
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제 1 강연장 발표 초록

Chemical Tools to Explore the "Hidden" Protein Phosphorylations

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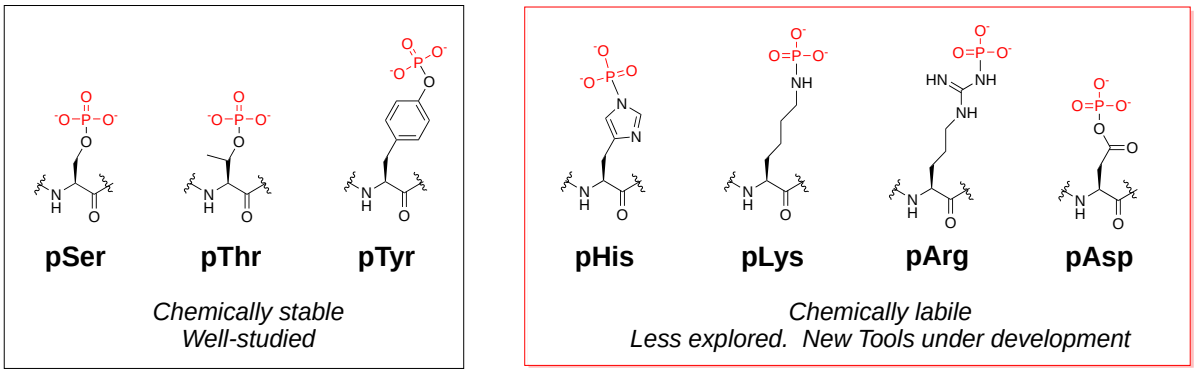
Protein phosphorylation is one of the most important post-translational modifications (PTMs), and the responsible kinases and phosphatases are important drug targets. Most of the current phosphorylation research focuses on pSer, pThr, and pTyr. In contrast, we are investigating non-canonical types of protein phosphorylation, such as phosphohistidine (pHis), phospholysine (pLys), phosphoarginine (pArg), and phosphoaspartate (pAsp). Despite their crucial roles in cell signaling and metabolism, these phosphorylations have remained unexplored, mainly due to the chemical instability and lack of research tools. Herein we will discuss our progress in developing chemical tools to study these phosphorylations, with an emphasis on arginine phosphorylation.



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기정민

조교수, 부교수: 울산과학기술원 화학과 (2014~현재)
연구분야: Chemical biology, protein phosphorylation, drug discovery
홈페이지: https://kee-lab.org

Stereoselective Synthesis of (*E*)- and (*Z*)-α-Silyl-α,β-unsaturated Amides with DIBAL-H and Isocyanates

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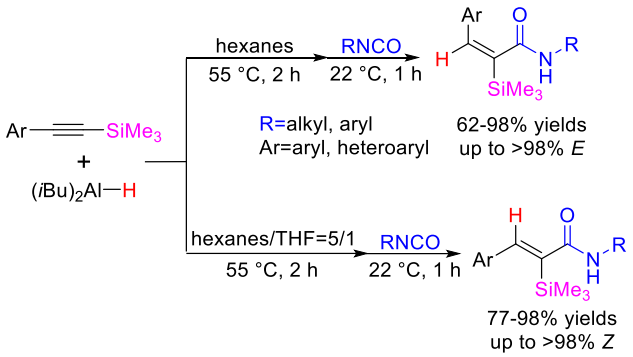
Conjugate amides have played important roles in various functional materials, drugs, and organic synthesis. Conventional method for the preparation of α,β-unsaturated amides is the coupling reaction of amines and activated carboxylic acid derivatives. However, this method has the lack of control over the regio- and stereoselectivity of acrylamides. Moreover, bulky amines are troublesome for the desired transformation due to the steric hindrance. We present the alternative synthetic protocol of (*E*)- and (*Z*)-silyl acrylamides through stereo- and regioselective hydroalumination of Si-substituted arylacetylenes and successive stereospecific nucleophilic addition of vinylaluminum to isocyanates. To the best of our knowledge, this is the first example of *E*- or *Z*-controllable hydroamidation reactions of alkynes. Stereoselectivity of hydroalumination was controlled by the use of coordinating solvent, tetrahydrofuran. Non-coordinating solvent, hexanes, led to the isomerization of Si-substituted vinylaluminum intermediate. In contrast, the mixture of hexanes and tetrahydrofuran as solvent inhibited it to generate >98% *Z* products. Based on the optimized condition, we checked the broad scopes of aryl/alkyl isocyanates and Si-tethered arylacetylenes. To demonstrate the synthetic applications, we conducted the transformation of C–Si bond into C–X (X= Br, I), C–H or C–C bond. Gram-scale synthesis was also demonstrated without any hurt of efficiency and stereoselectivity. Additionally, SiO_2 chromatography was not required for the isolation of the desired in gram-scale synthesis.



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정병혁

조교수, 부교수: DGIST 기초학부/신물질과학(2014~현재)
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홈페이지: https://sites.google.com/site/byunghyuckjung/home

Synthetic Studies of Natural Products: Curcusones and Mechanistic Elucidation of an Unexpected Rearrangement

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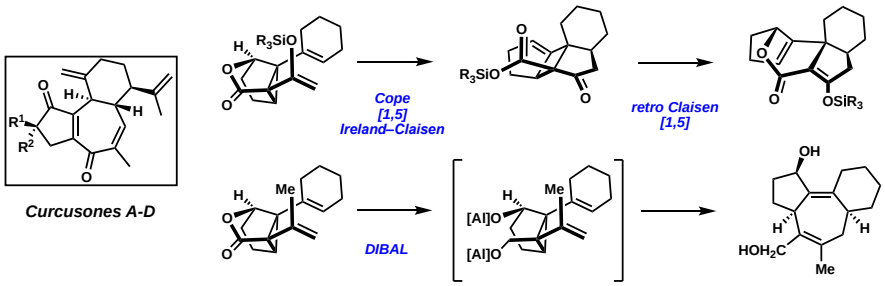
Curcusone C is tricyclic diterpenoid natural product isolated from *Jatropha curcas* that exhibits potent biological activity and features a 2,3,7,8- tetrahydroazulene-1,4-dione moiety. Synthetic approaches toward a tricyclic core of curcusones A-D via Suzuki coupling, intramolecular cyclopraopanation, and a key divinylcyclopropane rearrangement will be presented. Progress of our synthesis was repeatedly challenged by the highly substrate-dependent cyclopropanation step, which we were able to overcome by choice of substituents on the six-membered ring fragment.
During our investigation toward the synthesis of curcusones A–D, we discovered an unexpected thermal rearrangement of a divinylcyclopropane to the product of a formal Cope/1,3-sigmatropic shift sequence. Since thermal 1,3-sigmatropic shift is forbidden, computational studies were applied to explore the mechanism. Eventually, we were able to elucidate thermally allowed pericyclic rearrangements cascade of Cope rearrangement/ 1,5-sigmatropic silyl shift/ Claisen rearrangement/ retro-Claisen rearrangement/ 1,5-sigmatropic silyl shift.



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이충환

조교수: 가천대학교 화학과(2021~현재)
연구분야: synthetic methodology, organic electronic materials, natural product synthesis
홈페이지: https://sites.google.com/view/cwleegroup/

New Photodynamic Therapy Methods and Applications Selective for Two-Photon Excitation

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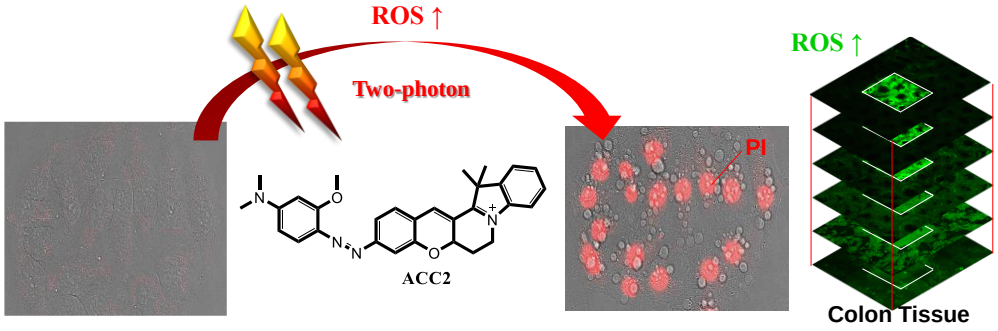
A photosensitizer (PS) is essential for photodynamic therapy (PDT) and generates reactive oxygen species (ROS) when irradiated with light. Cell damage is induced by overexpressed ROS, which ultimately leads to apoptosis.[1] PDT can overcome the limitations of existing therapies by having advantages such as non-invasive treatment, a simple treatment process, and minimization of drug resistance. Two-photon excitation (TPE) is an effective way to make these PDTs more useful. Since TPE uses low energy light corresponding to the near infrared (IR) (700–950 nm) region as a light source, it can be applied deep into the tissue to be treated.[2] In addition, TP-PDT has the advantage of minimizing photodamage to healthy tissue and being able to perform only at a specific location requiring treatment.[3] If a PS that selectively responds to TPE can be developed, its utility is expected to be very high.

In response to this requirement, we developed cyclized-cyanine derivatives PS containing an azo group (ACC2). In addition, it was confirmed that recently, a polyethylene glycol structure was additionally introduced into the TP-PS to increase the cell staining ability and increase the therapeutic effect (PEG-ACC2). These dyes showed higher ROS generation ability in two-photon excitation than in one-photon excitation. In the results of cell imaging experiments using PEG-ACC2, it was confirmed that effective PDT performance was shown even at low concentrations and low number of scans. Therefore, we would like to present a novel TP-selective PDT method through PEG-ACC2.



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임창수

조교수: 아주대학교 화학과 (2016~현재)
연구분야: Two-photon fluorescent probes, Two-photon microscopy imaging, Cancer early diagnosis and photodynamic therapy
홈페이지: https://chem.ajou.ac.kr/chem/member/member02.jsp

Acyl Fluoride Generation Promoted by Hypervalent Iodine(III) Reagents: Effective Method for Hindered Amide-Bond Formation

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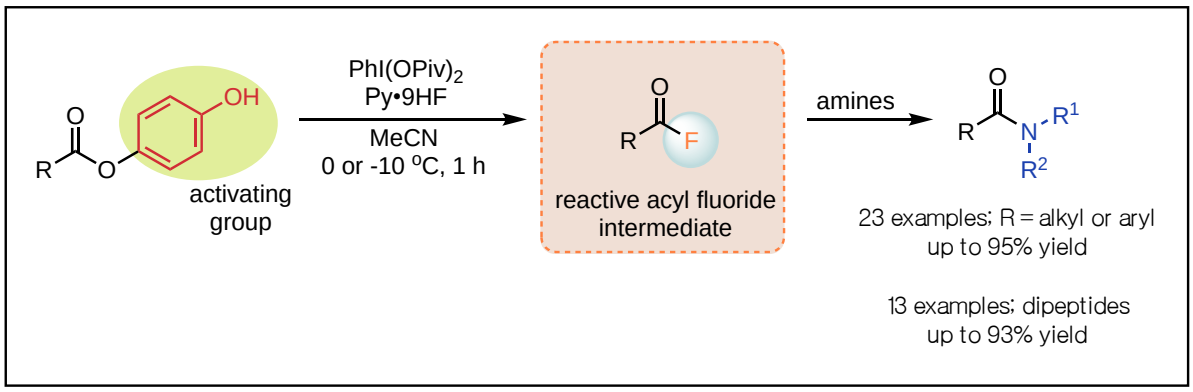
Amide-bond, one of the fundamental functional group in organic chemistry, is ubiquitous in bioactive compounds such as natural products, drugs, and agrochemicals and has been employed to develop their activities. In particular, amides bearing sterically bulky substituents in α-position are highly desirable in medicinal chemistry as the incorporation of a bulky peptide bond in a molecule provides the drug with a sustainable in vivo pharmacological effect. However, this area remains underexplored due to the difficulties associated with the preparation of hindered peptides using conventional methods. Therefore, development of highly efficient method for amide-bond formation has become a topic of great scientific interest in modern organic chemistry. Here we report a new amide-formation from various esters that possess a phenol moiety as a potential activating group (PAG) at the ester residue. The PAG was activated by hypervalent iodine(III) promoted dearomatization of phenols under mild conditions and highly reactive acyl fluoride intermediates were generated efficiently using a pyridine-hydrogen fluoride complex. Subsequent transformation of the resulting acyl fluoride with amines provided corresponding amides in high yield (up to 95% yield, 23 examples). Employing alcohol as a nucleophile, furthermore, products of the transesterification were obtained in high yield (up to 95% yield). With our new protocol, peptide synthesis including sterically hindered one was achieved as well (up to 93% yield, 13 examples). Synthetically, smooth formation of amide-bond under mild conditions was accomplished successfully. This amide coupling protocol, consequently, can be expected to find broad synthetic applications in de novo synthesis and late-stage functionalization strategies.



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이효준

조교수: 군산대학교 화학과(2020~현재)
연구분야: Asymmetric Organocatalysis, Development of New Synthetic Methods, Hypervalent Iodine(III) Chemistry

Enzyme-Catalyzed Self-Assembly of Peptide for Selective Inhibition of Cancer Cells

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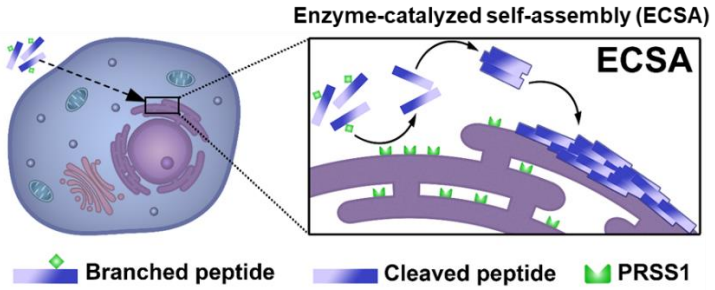
Molecular self-assembly is ubiquitous in living systems, leading to the formation of innumerable biological complexes spatiotemporally regulated. Inspiring by nature, the novel methodology, enzyme-catalyzed self-assembly, has been developed for the spatiotemporal control of self-assembly. It also enables molecular self-assembly to be spatiotemporally regulated in cancer cellular milieu, leading to the formation of assemblies at the specific positions of cancer cells. The PRSS1-catalyzed self-assembly of peptide derivatives facilitates the selectively targeting of endoplasmic reticulum(ER) in OVSAHO cancer cell, promising the application in targeted cancer therapy. This simple strategy for molecular self-assembly controlled in cellular milieu will advance chemical manipulability of cell viability as well as development of molecular targeted cancer therapy.



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김범진

조교수: 울산대학교 화학과(2020~현재)
연구분야: bioorganic chemistry, peptide self-assembly, biomaterials
홈페이지: https://sites.google.com/view/bjkimgroup

Cooperative Pd(0)/Rh(II) Dual Catalysis for the Synthesis of Heterocyclic Compounds

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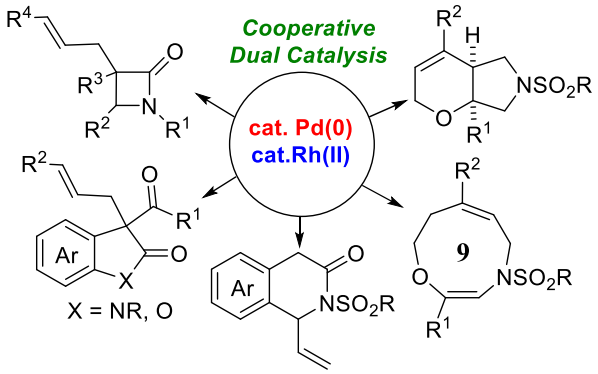
Cooperation of two-different catalytic cycles in one-pot is a highly attractive and challenging synthetic strategy. Despite considerable recent advances, the dual catalytic systems composed of two-different transition-metals are still limited, which may attribute in part to the inherent difficulty in insuring of redox compatibility between the catalysts and balanced kinetics, avoiding catalyst deactivation.[1] In this regards, we have recently demonstrated for the first time the redox-compatibility between Pd(0) and Rh(II) catalysts through the synergistic cooperative Rh(II)/Pd(0) dual catalytic reaction between N-sulfonyl-1,2,3-triazoles and allylic substrates.[2] During our continuing studies on cooperative dual transition-metal catalysis, it was found that the cooperative Pd(0)/Rh(II) dual catalysis is of particularly useful for the constructions of four-nine membered heterocyclic moieties.[3]



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New Approach for Live Cell Distinction through Lipid (LOLD)

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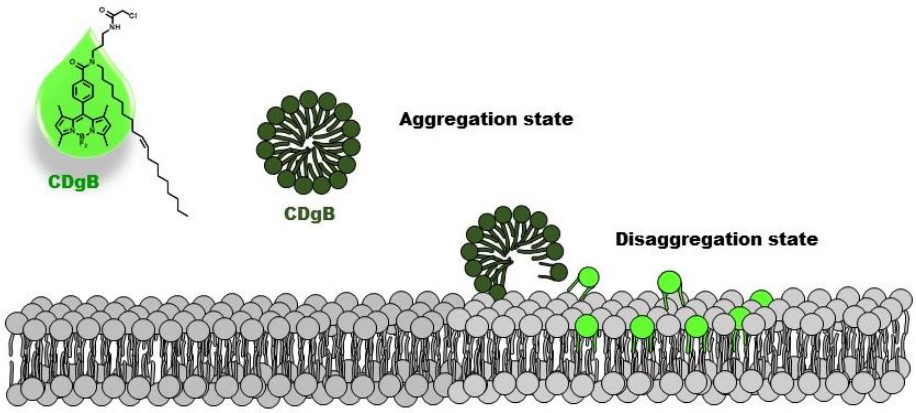
Distinction of cell types in multicellular organism is the most important first step to understand the complex cell community and control their regulation. The conventional approach of cell distinction is through magic bullet molecule for specific biomarker in each cell. Proteins and carbohydrates have been the most popular binding targets for fluorescent probe. Here I report a new approach of cell distinction through the lipid composition on plasma membrane. In addition to Protein Oriented Live-cell Distinction (POLD) and Carbohydrate Oriented Live-cell Distinction (COLD), Lipid Oriented Live-cell Distinction (LOLD) provides totally different dimension of Cell discriminating power for analyzing complex cell system, such as immune system. The first B cell selective probe CDgB and LOLD mechanism, elucidated from T and B lymphocyte distinction campaign, has been applied to the analysis of developmental stages in immune cell maturation.



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Peptide Nucleic Acid-based Hybridization Chain Reaction (HCR) for Imaging of Cellular Targets

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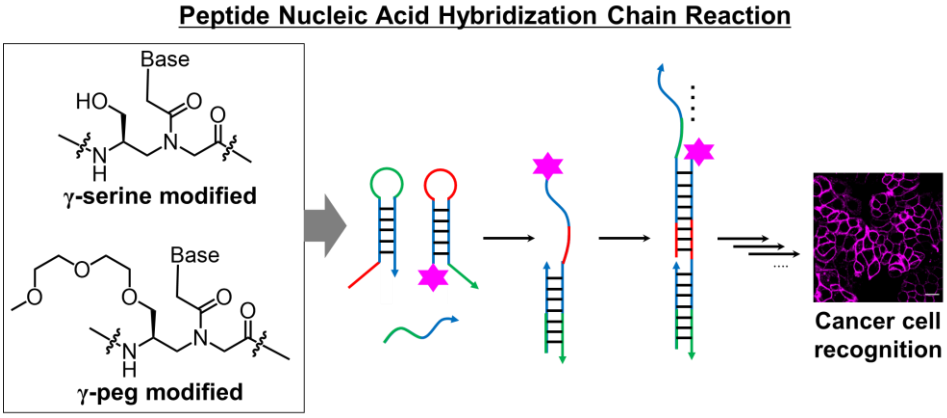
Oligonucleotides are an attractive platform for the construction of programmed molecular systems with emerging functions such as logic-gated operations and enzyme-free amplifications. One of the major achievements for amplification is DNA or RNA hybridization chain reaction (HCR) where two metastable hairpins form long stretches of duplexes by alternative hybridization in the presence of target nucleic acids. Owing to its high amplification efficiency and multiplexed designs, HCR systems have been utilized as powerful tools for biosensing and diagnostic applications. However, canonical DNA HCR uses long DNA sequences for hairpin metastability, which increases cost and decreases signal density, and thus a minimal version of HCR is required. Herein, we report a minimal HCR system enabled by γ-serine or γ-peg modified peptide nucleic acids (PNAs). A designed system made of 5-mer stem and 5-mer loop/toehold hairpins afforded >10-fold of fluorescence amplification in 2 hours. This HCR design was applied to distinct visualization of a cancer biomarker, carbonic anhydrase IX (CA IX), in live cells.



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김기태

조교수: 충북대학교 화학과(2020~현재)
연구분야: Nucleic acid chemistry, Fluorescence sensing and imaging, DNA nanotechnology
홈페이지: http://sites.google.com/view/ktkim-lab/

Visible-Light Photoredox-Catalyzed Selective Transformation of Oxaziridines into Nitrones and Amides

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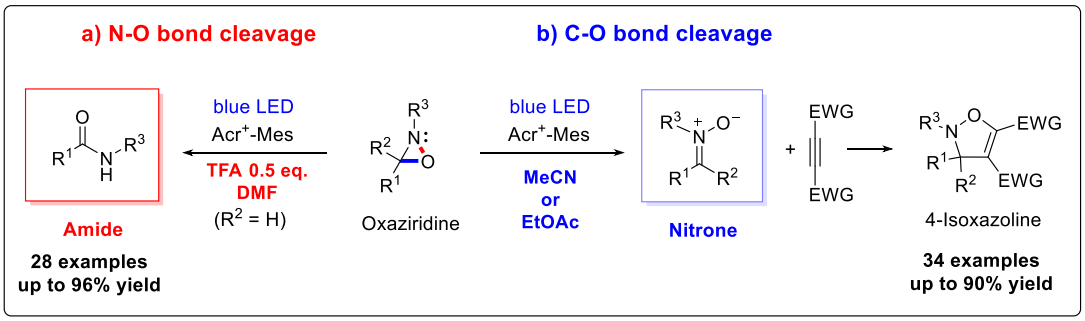
Email: woosk@ulsan.ac.kr

Visible light-mediated photoredox catalysis is an emerging research area in organic synthesis since visible light provides an inexpensive, infinite, and clean energy source. Recently, we developed new method for selective generation of nitrones and amides from oxaziridines by visible light photoredox catalysis. First, we developed a greener method for preparation of 4-isoxazolines in a visible light photoredox-catalyzed [3+2] cycloaddition of oxaziridines with alkynes (Scheme 1, b).[1] This method involves in situ generation of nitrones from oxaziridines by SET. The [3+2] cycloaddition tolerates various functional groups and provides good to excellent yields. A mechanistic study suggests that the reaction involves photoredox catalyzed in situ generation of a nitrone from the oxaziridine by SET. Second, we developed selective transformation of oxaziridines into amides using TFA as additive and DMF as solvent. The amide formation tolerates various functional groups and provides good to excellent yields. We explained this selectivity through mechanism study using DFT calculations and controlled experiments. Herein, the recent our works will be discussed in detail.



Scheme 1. Photoredox-catalyzed selective transformation of oxaziridines into nitrones and amides

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우상국

조교수, 부교수: 울산대학교 화학과(2013~현재)
연구분야: Organic synthesis, Synthetic methods, Photoredox chemistry
홈페이지: https://sites.google.com/site/wooresearchgroup/

Manganese-Catalyzed Late-Stage C–H Diversification of Peptides: Modular Synthesis of Fluorogenic Probes

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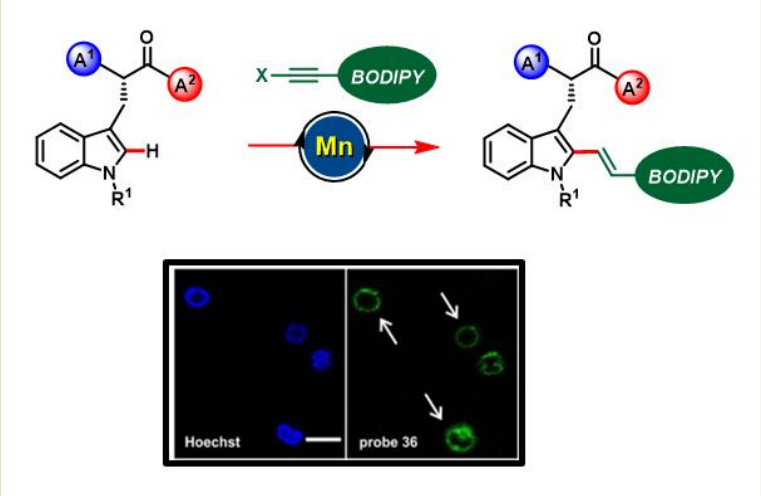
Bioorthogonal late-stage diversification of amino acids and peptides bears enormous potential for drug discovery and molecular imaging. Despite major accomplishments, these strategies largely rely on traditional, lengthy prefunctionalization methods, heavily involving precious transition-metal catalysis. Herein, we report on a resource-economical manganese (I)-catalyzed C–H fluorescent labelling of structurally complex peptides ensured by direct alkynylation and alkenylation manifolds. This modular strategy sets the stage for unravelling structure-activity relationships between novel fluorophores towards the rational design of new BODIPY fluorogenic probes for real-time analysis of immune cell function.



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손종우

조교수: 동아대학교 화학과(2020.09~현재)
연구분야: synthetic organic chemistry, late-stage C–H modification of peptides, and heterocyclic chemistry
홈페이지: https://sonorganic1.wixsite.com/jongwooson

Utilization of the *N*-silyl Enamine Intermediate from *N*-Heteroarene: Synthesis of Cyclic Amidines and Bicyclic Pyrazolidine Derivatives

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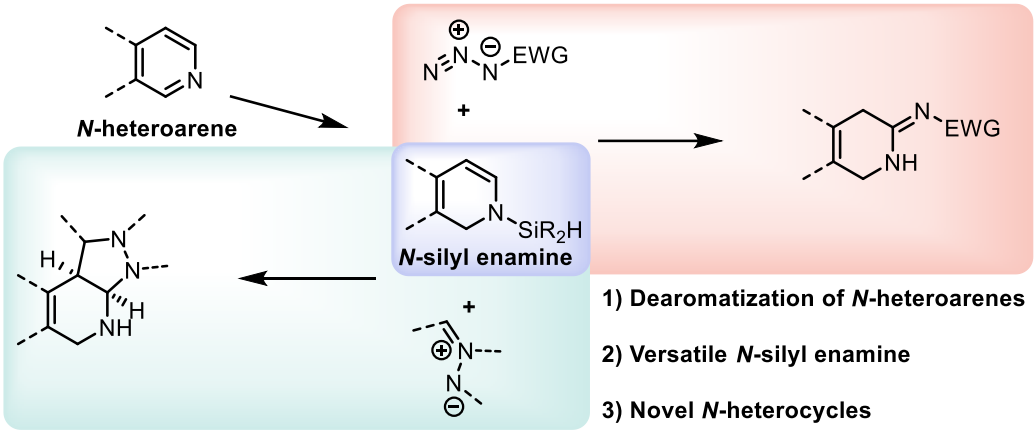
Regioselective dearomatization of the readily available *N*-heteroarenes is an emerging strategy to obtain complex molecules. Especially, $B(C_6F_5)_3$ catalyzed dearomative hydrosilylation of the *N*-heteroarenes has been studied actively. However, due to the intrinsic unstability of the N–Si bond, the utility of the partially reduced *N*-silyl enamine intermediate from the mono-hydrosilylation of the *N*-heteroarene has been rarely reported. In this context, our group recently developed a methodology to synthesize the cyclic amidine by using *in situ* utilization of the *N*-silyl enamine with organic azide.[1] [3 + 2] cycloaddition and rearrangement involving hydride shift resulted in (*Z*)-selective cyclic amidine. The substrate scope has been widely expanded from quinolines to isoquinolines and pyridines[2] with various class of electron withdrawing organic azides. Furthermore, we recently discovered a reactivity of the *N*-silyl enamine toward azomethine imine which could achieve novel bicyclic pyrazolidine skeleton.



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정시원

조교수: 목포대학교 화학과(2018~현재)
연구분야: [3 + 2] cycloaddition, *N*-heterocycles, $B(C_6F_5)_3$
홈페이지: https://sites.google.com/view/jounglab

α-C-H Bond Functionalization of Unprotected Cyclic Amines via Transient Imines

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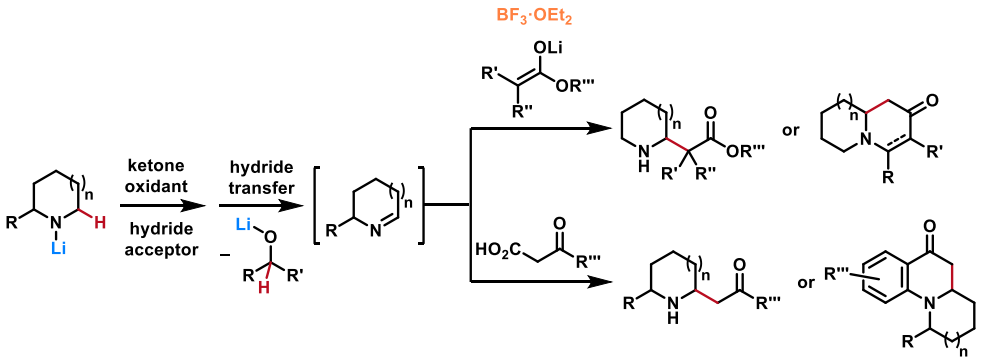
Substituted cyclic amines are key constituents of important pharmaceutical drugs. State-of-the-art approaches access such heterocycles via the functionalization of C–H bonds. However, known approaches suffer from limitations, which involve the incompatibility with an N–H bond and the need for protecting and/or directing groups.

A new advance in this area utilizes *N*-lithiated cyclic amines and a simple ketone oxidant to provide transient imines which can be functionalized with various nucleophiles. We have achieved the alkylation of transiently generated imines with enolates in the presence of Lewis acid to provide valuable β-amino ketones.[1] The resulting α-alkylated cyclic amines could be further functionalized via condensation or intramolecular heteroconjugate addition by taking advantage of the unprotected amine moiety. The alkylation of transiently generated imines with β-ketoacids under mild decarboxylative conditions provided β-amino ketones with unprecedented ease.[2] Importantly, regioselective α'-alkylation was achieved for substrates with existing α-substituents. Further substrate diversification was achieved by combining decarboxylative alkylation with a subsequent S_NAr step in a single operation to provide polycyclic dihydroquinolones.



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김재현

조교수: 강원대학교 약학대학 (2020~현재)
연구분야: total synthesis, antibacterial drugs, sphingolipid metabolism modulators
홈페이지: https://sites.google.com/view/jhkimlab

Directed and Non-Directed Annulative π-Extension Reactions

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C–H arylation potentially provides a concise synthetic strategy while eliminating the need for pre-functionalization of substrates. However, the precise control of the site-selectivity and multiple catalytic cycle operations are hurdles to step-efficient access to polyaromatic hydrocarbons (PAHs). We disclosed palladium-catalyzed 2-fold C–H activation approaches to afford functionalized triphenylene frameworks from DG-bearing arenes. This method offers a distinct platform for one-step annulative π-extension (APEX) by employing cyclic diaryliodonium reagents. Although fused cyclic substrates, heteroarenes, and modified arenes have been utilized in APEX chemistry, a nondirected C–H arylation of benzene and its derivatives to access two-dimensional honeycomb networks has remained a difficult issue owing to the low intrinsic reactivity and site-selectivity in the absence of a chelating group. We also demonstrated the palladium-catalyzed nondirected C–H annulation approach using simple arenes. We expect that this study can provide straightforward bottom-up synthetic routes for PAHs.

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홍성유

조교수, 부교수: 울산과학기술원, 화학과 (2010.11~현재)
연구분야: metal-catalyzed annulation, (cyclo)addition reactions
홈페이지: https://home.unist.ac.kr/professor/syhong/index.html

Highly Enantioselective Synthesis of Trisubstituted Epoxides: Catalytic Asymmetric Darzens-type Epoxidation of Diazoesters

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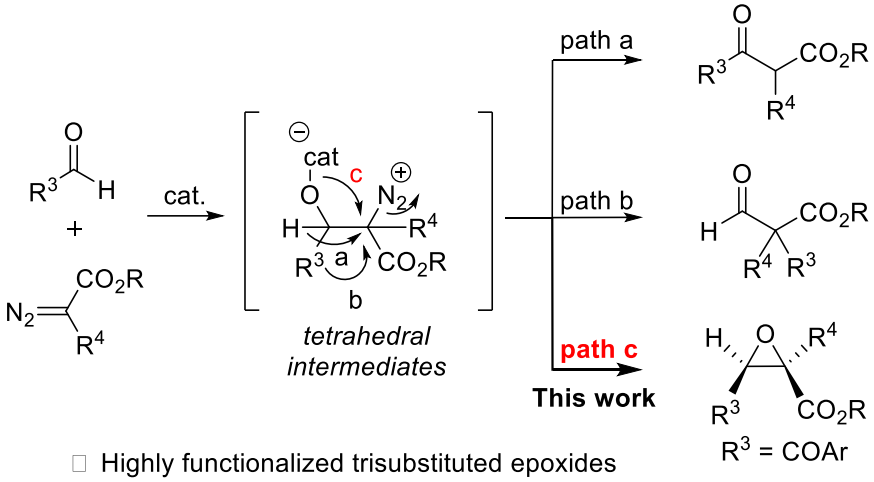
Optically active α,β-epoxy carbonyl compounds are versatile building blocks for the synthesis of biologically active molecules and powerful key intermediates in a broad array of applications for asymmetric synthesis. Accordingly, numerous efforts have been dedicated to efficient preparation of these compounds. Among the various synthetic methods, asymmetric Darzens condensation and Corey-Chaykovsky reaction using a sulfur ylide are a particularly powerful approaches in terms of direct asymmetric conversion of carbonyl compounds into epoxides. However, except for a few examples of catalytic methods, synthetic application of these reaction depends on chiral auxiliary methods or chiral reagent-mediated approaches.

Recently, our group reported highly enantioselective catalytic tandem reactions of diazo compounds with the chiral oxazaborolidinium ion (COBI) as a Lewis acid catalyst. After forming tetrahedral intermediate through nucleophilic addition of diazo compounds into aldehyde, H-migration (Roskamp reaction, path a) and C-migration (path b) led to the construction of optically active β-keto ester and the all-carbon quaternary aldehyde, respectively. In this talk, I will present a highly asymmetric catalytic method for synthesis of trisubstituted α,β-epoxy carbonyl compounds in Darzens-type reaction (path c).



- Highly functionalized trisubstituted epoxides
- Excellent stereoselectivity (>20:1 dr, up to >99% ee)

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류도현

조교수, 부교수, 정교수: 성균관대학교 화학과(2005~현재)
연구분야: Asymmetric catalyst, Synthetic methodology, Total synthesis of natural products and functional organic materials
홈페이지: https://swb.skku.edu/npsl/index.do

P- and S-Ylides for C–H Functionalization of *N*-Heterocycles

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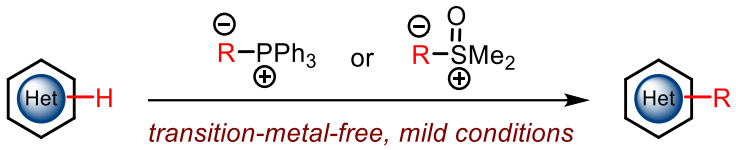
Wittig reaction, which is based on the reaction of an aldehyde or ketone with a phosphonium ylide, is ranked among the most important reactions for C–C bond formation. Phosphonium ylides have also been used as C nucleophiles in Michael addition and other alkylation reactions. Moreover, phosphonium salts have been applied to organocatalytic Mannich-type processes to afford aza-Morita–Baylis–Hillman adducts. Since the pioneering work of Johnson, Corey, and Chaykovsky in the 1960s, sulfur ylides have been extensively utilized for cyclization reactions with electron-deficient π-unsaturated compounds to afford a wide range of carbocyclic and heterocyclic compounds. Mechanistically, the nucleophilic addition of sulfur ylides into π-unsaturated compounds such as carbonyl, imine, and α,β-unsaturated moieties leads to the formation of betaine intermediates, which are decomposed by O, N, and C anions via intramolecular nucleophilic substitution. However, there are no reports on C–H alkylation reactions of (hetero)aromatic compounds using phosphonium and sulfonium ylides to date.

Recently, we explored the unprecedented reductive alkylation of pyridine and quinoline-*N*-oxides using Wittig reagents as novel aromatic alkylation surrogates.[1,2] In addition, we described the C2-selective C−H methylation of heterocyclic *N*-oxides with sulfonium ylides.[3] Moreover, we developed the C(sp^2)–H alkylation of iminoamido heterocycles as nucleoside base analogues with sulfur ylides as alkylating agents under aqueous conditions.[4]

Herein, we demonstrate the transition-metal-free and direct C–H alkylation of various *N*-heterocycles using phosphonium and sulfonium ylides. The applicability of the developed protocol is showcased by the late-stage alkylation and sequential transformations of complex drug molecules.



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김인수

조교수, 부교수, 교수: 성균관대학교 약학과(2009~현재)
연구분야: C–H functionalization, heterocycle synthesis, total synthesis, drug discovery(anticancer, antidiabetes)
홈페이지: http://pharmasyn.skku.edu/intex.asp

Synthesis of Triscarbene-Modified Iridium Catalysts and Their Application to β-Alkylation of Alcohols

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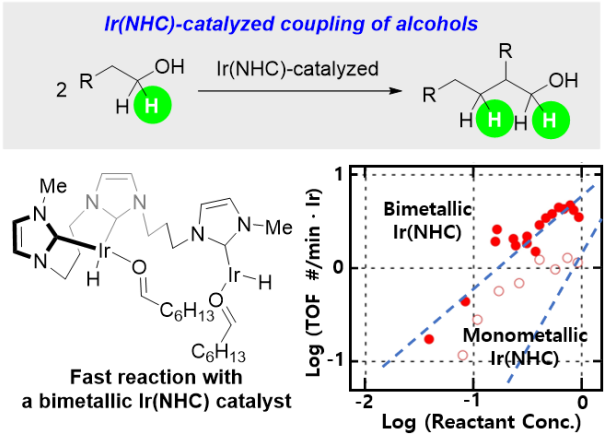
Transition metal catalysts modified with polydentate *N*-heterocyclic carbene (NHC) have been utilized in homogeneous catalytic reactions. The unique electronic and structural effects of polydentate NHC ligands provide unexpected catalytic properties. Our research group has been investigating new organometallic complexes. In particular, triscarbene-coordinated transition metal complexes have been synthesized and explored in various organic transformations. In this presentation, we present the synthesis and characterization of new triscarbene-coordinated iridium complexes (monometallic and bimetallic complexes) and their application in the β-alkylation of alcohols; dimerization of primary alcohols (Guerbet reaction), cross-coupling of secondary and primary alcohols, and intramolecular cyclization of alcohols. Mechanistic studies of Guerbet reaction, including kinetic experiments, mass analysis, and density functional theory (DFT) calculation, were conducted to explain the fast reaction promoted by bimetallic catalysts and the dramatic reactivity increase of monometallic catalysts at the late stage of the reaction.



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장혜영

교수: 아주대학교 화학과 (2006~현재)
연구분야: green catalysis, CO_2 & CO utilization, sustainable reactions
홈페이지: https://sites.google.com/ajou.ac.kr/ajouom/home

Synthesis of Zwitterionic L-DOPA and its Applications to Virus Immunoassay/Medical Implant

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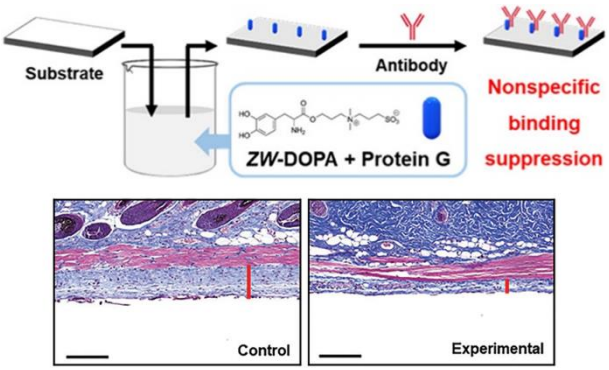
Inspired by mussel's adhesive proteins, polydopamine chemistry has served as one of the simplest and versatile approaches to functionalize surfaces. It was reported that catechol and amine groups of 3-(3,4-dihydroxyphenyl)-L-alanine (L-DOPA) in the adhesive proteins play important roles in the exceptional adhesion capability of mussels. While dopamine and the catechol-conjugated polymers have been widely used for many different applications including adhesive hydrogels, antibacterial coatings, cell encapsulation, there has been little study on the synthesis of functional L-DOPA derivative. Herein, we synthesized a zwitterionic L-DOPA (*ZW*-DOPA) as a non-biofouling material, and demonstrated its applications to influenza virus immunoassay and medical implant. Using the combination of *ZW*-DOPA and protein G, we developed a versatile platform that can not only immobilize antibody optimally but also suppress the non-specific bindings. *ZW*-DOPA/protein G-coated substrate could be utilized to detect influenza A/CA/07/2009 (pH1N1) by the naked eye and with surface-enhanced Raman scattering measurements. The non-biofouling efficacy of *ZW*-DOPA was further applied to suppress capsule formation on silicone implant. Capsule formation was significantly inhibited by *ZW*-DOPA coating *in vivo* and the differentiation of fibroblasts into myofibroblasts was also significantly inhibited. Considering the ease of use and universal coating capability, we believe that *ZW*-DOPA can be used as an anti-fibrotic and non-biofouling material for various biomedical tools and devices.



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조우경

조교수, 부교수: 충남대학교 화학과(2013. 9~현재)
연구분야: Biomaterials, nature-inspired organic materials, functional coatings
홈페이지: https://sites.google.com/site/wkchogroup/

DAST-mediated C−C Bond Cleavage of Activated Carbonyl Compounds

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The Beckmann rearrangement (BKR) is one of the most basic transformations handled in college-level organic chemistry textbooks. Discovered by Ernst Otto Beckmann in 1886, it is a rearrangement of alkyl- or aryloxime functionality into secondary amides. The reaction generally occurs under acidic conditions or in the presence of activating reagents that can make the oxime-hydroxyl as a good leaving group. Meanwhile, the BKR often competes with the Beckmann fragmentation (BKF); the pathway selection between two reactions is reliant on the structure of substrates and reaction conditions. In case of BKFs, there are two types of BKF products; one is obtained from *β*-hydrogen elimination to release alkene and nitrile and the other is derived from nucleophilic attack at α-position of oximes to generate C–Nu bond and nitrile. Both process should involve oxime-hydroxyl activation and a subsequent dehydroxylation by the relevant electron pair flow.

During our research program to search novel agrochemical scaffolds and the efficient functionalization of small heterocyclic compounds, we developed a new protocol for synthesis of highly useful acylation reagents. The design is based on the BKR that uses activated carbonyl compounds as substrates and DAST (diethylaminosulfur trifluoride) as a dual role reagent. The synthesis plan and outcome will be shortly discussed in this talk.

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임희남

선임연구원, 한국화학연구원 친환경신물질연구센터 (2016.11-2021.02)
조교수, 영남대학교 화학생화학과 (2021.03-현재)
연구분야: Discovery of novel agrochemical scaffolds, Synthetic Methods, Total Synthesis & Drug Discovery

Chemistry of Amyloids and Catechols

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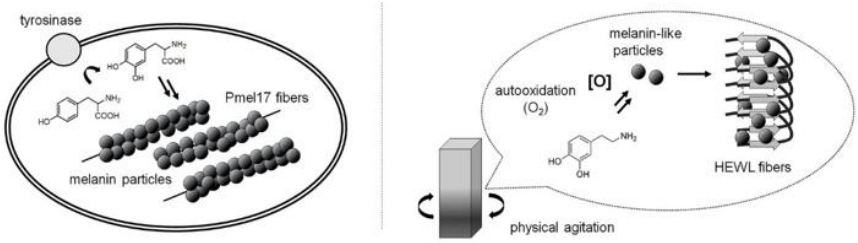
Catechol derivatives (e.g., catechols, catecholamines, and flavonoids) have been frequently linked to amyloid—a protein-aggregated fibrillar structure rich in cross-β-sheet—and its related diseases as a potential cure. They were effective in morphologically remodeling amyloid fibers or in altering the kinetics of their formation. One remarkable example is epigallocatechin-3-gallate (EGCG; a major component in green tea extract), which is currently involved in multiple clinical trials, since it has been reported to be capable of remodeling amyloid fibrillar structures and neutralizing their cytotoxicity.
The nature of catechol-amyloid interaction, however, is beyond a simple unilateral regulation of one by another, but it is mutual and multifaceted. At oxidative conditions, catechol derivatives (particularly catecholamines) spontaneously form heterogenous molecular complexes—often called 'melanin-like species'—composed of non-covalently associated oligomeric structures. A few clues suggested that such oxidative association of catechol derivatives may be critically regulated by amyloids. In melanogenesis, an amyloid fiber made of a melanosomal protein (Pmel17) is crucial for the formation of melanin (i.e., the oxidative association of dopamine). A currently accepted role of Pmel17 fibers is capturing toxic intermediates during the process of melanogenesis, but their actual roles are likely multifaceted and underestimated. We previously shown that amyloid fibers made of various proteins (sub-domains of Pmel17 and even a biologically irrelevant protein (hen egg white lysozyme; HEWL)) have multifaceted functions on the oxidative association of dopamine, such as accelerating the association process and altering the materials properties of melanin-like species greatly by forming composite materials together. A summary of our recent approaches to elucidate chemistry between amyloids and catechol derivatives will be given.



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강경태

조교수: 경희대학교 응용화학과(2016~현재)
연구분야: peptide chemistry, catechol chemistry, supramolecular functionality
홈페이지: http://kkang.khu.ac.kr

Development of Chiral Pyridine-Dihydroisoquinoline Ligands

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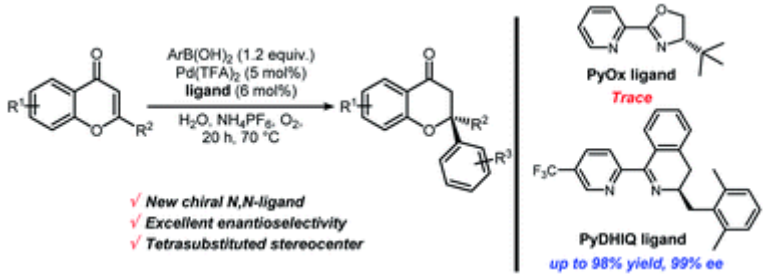
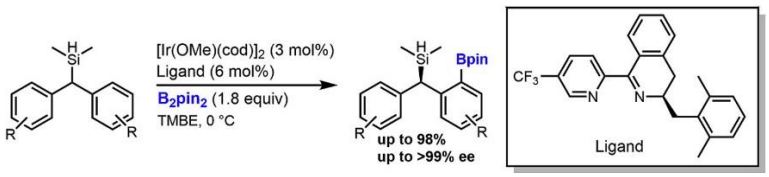
Highly enantioselective conjugate addition reactions of arylboronic acids to 2-substituted chromones catalyzed by palladium complexes with new chiral Pyridine-Dihydroisoquinoline (PyDHIQ) ligands have been developed.[1] These reactions provide highly enantioselective access to chromanones containing tetrasubstituted stereocenters. Various arylboronic acids and 2-substituted chromones can be used in the catalytic reaction to afford the chiral tetrasubstituted chromanones in good yields and excellent enantioselectivities (25 examples, up to 98% yields, up to 99% ee). In addition, *e*nantioselective C(sp^2)−H borylations of diarylmethylsilanes were catalyzed using iridium complexes with chiral pyridine-dihydroisoquinoline (PyDHIQ) ligands.[2] High enantioselectivities (up to >99% ee) were observed for various substrates. A gram-scale synthesis was achieved using 1 mol% of the catalyst to afford a 91% yield of the desired chiral borylated organosilane product with >99% ee. Our ongoing efforts to develop chiral N-Heterocyclic carbene ligands will also be discussed in this presentation.



Chem. Sci. **2020**, *11*, 4602-4607



Tetrahedron **2021**, *79*, 131811

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홍석원

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부교수: GIST 신소재공학부 (2012~2016)
부교수, 교수: GIST 화학과 (2016~현재)
연구분야: Asymmetric Catalysis, N-Heterocyclic Carbene Ligands, Sustainable Catalysis
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제 2 강연장 발표 초록

Photo-activation Approach to Spatio-temporal Mapping for Biomolecule Interactions in Complex Biological Environment

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Protein-protein interactions (PPIs) trigger a wide range of biological signaling pathways that are crucial for biomedical research and drug discovery. Various techniques have been used to study specific proteins, including affinity chromatography, activity-based probes, affinity-based probes and photo-affinity labeling (PAL). PAL has become one of the most powerful strategies to study PPIs. Traditional photo-crosslinkers are used in PAL, including benzophenone, aryl azide, and diazirine. Upon photoirradiation, these photo-crosslinkers (Pls) generate highly reactive species that react with adjacent molecules, resulting in a direct covalent modification. Recently, we report the first rational design of a photo-crosslinking BODIPY fluorophore (pcBD) and its biological application for biomolecule labeling. As a photosensitizing functional motif, an aryl ketone group was incorporated into the BODIPY fluorophore, and a series of proteins were labeled by pcBD compounds upon UV irradiation. In order to investigate protein–protein interactions in a protein mixture, amino-functionalized pcBD was prepared and covalently attached to a ubiquitin ligase binding peptide. Upon UV irradiation, we could successfully visualize the substrates in the total lysate. These results provided a proof of concept for spatially controllable tagging via photo-activation of the pcBD scaffold and demonstrated its potential usage for in situ labeling applications. In addition to photo-affinity fluorophore scaffold, we also examined series of photo activatable functional groups, including tetrazole. Photolysis of tetrazoles to nitrile imines are extremely rapid and efficient process and the light-induced tetrazole-alkene 1,3-dipolar cycloaddition (also known as tetrazole photoclick chemistry) was first reported as a bioorthogonal reaction in 2008 by Lin's group. We explored the alternative use of the tetrazole photoclick reaction inspired by the high electrophilicity of nitrile imine species and revealed nucleophilic side chain of protein could generate chemical crosslinking. In this presentation, we will discuss another kinds of photo-activatable crosslinking approach to investigate proximity of two biomolecules in complex biological environment.

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이준석

책임/선임/연구원: 한국과학기술연구원 (2010 ~ 2020)
조/부교수: KIST School UST (2013 ~ 2020)
부교수: 고려대학교 의과대학 약리학교실 (2021~현재)
연구분야: Multi-functional probes for proteomics, Host-pathogen interactions
홈페이지: https://leegroup.chembiol.re.kr

Electrochemically Driven Stereoselective Approach to *syn*-1,2-Diol Derivatives from Vinylarenes and DMF

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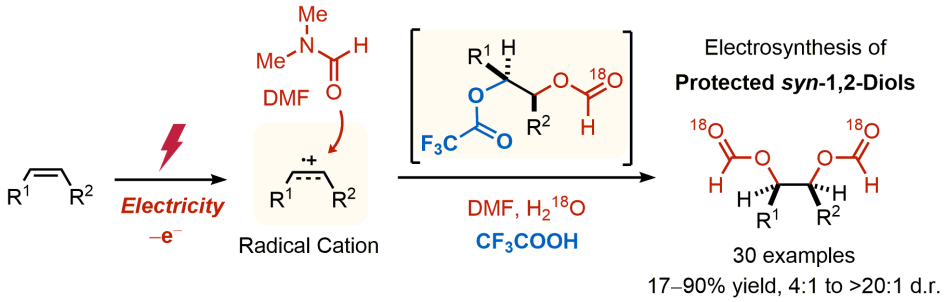
The dihydroxylation of alkenes is a fundamental and straightforward transformation for the preparation of 1,2-diols, which is widely used in the preparation of key intermediates in fragrances, pharmaceuticals and functional materials. Most of the precedent examples however still rely on the use of transition metals for the requisite redox process or otherwise require additional synthetic steps for the preparation of reaction mediators. In addition, an employment of a chemical oxidant system (e.g. hypervalent iodines) olefin leads to limited functional group compatibility. In this regard, we envisioned an electrochemical alkene oxidation as an ideal approach. Herein, we devised an electrooxidative strategy that grants access to formyl-protected *syn*-1,2-diols from vinylarenes and DMF. This reaction is initiated by the electrochemical oxidation of the alkene substrates followed by the nucleophile attack of DMF. Mechanistic studies imply that trifuoroacetate ion is presumably engaged in the nucleophilic capture of the carbocation intermediate, which gives rise to high syn-diastereoselectivity. A simple deprotection of formyl protecting groups from the dioxygenated product was also presented, highlighting synthetic utility of this electrochemical method toward a variety of 1,2-diols. We anticipate this electrochemical synthetic approach promoted by trifuoroacetic acid will be broadly applicable in further development of nucleophilic olefin functionalization reactions.



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김현우

조교수: 이화여자대학교 화학과 (2020~현재)
연구분야: Electrocatalysis for Organic Synthesis, Radical Redox Relay Catlaysis, Development of Organic-Based Energy Storage System
홈페이지: https://lexontkfu.wixsite.com/hyunwookimlab

Synthetic Studies toward the Total Synthesis of Arenaric Acid

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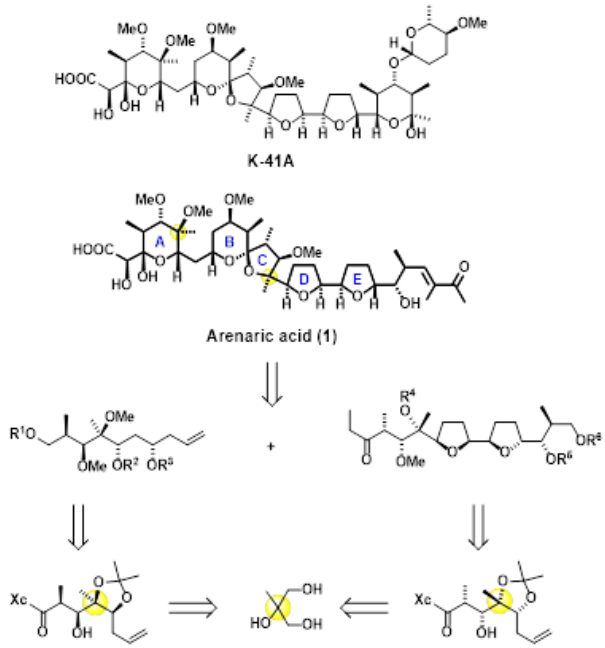
K-41A, isolated from Streptomyces hygroscopicus K-41 in 1979,[1] displays antibacterial activity against Gram-positive bacteria, anticoccidal activity and delayed toxicity for poultry. Antibiotic K-41A was converted to **1** by removal of amicetose moiety through microbial and chemical transformation.[2] Arenaric acid **1**, a naturally occurring pentacyclic polyether, was isolated from marine sediments, *Streptomyces sp.,* near the north San Diego in 1999.[3] Arenaric acid **1** has molecular formula of $C_{41}H_{68}O_{15}$, 19 asymmetric carbons, one spiroketal, 5 oxacycles and two tetrasubstituted carbon stereocenters. Toward the synthesis of structurally complex polyketide **1**, the stereocenters were installed by enantioselective desymmetrization, asymmetric allylations, diastereoselective aldol reactions and iodoetherification as key steps.



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이원철

조교수: 강원대학교 화학과 (2020~현재)
연구분야: natural product total synthesis, synthetic methodology, organic material synthesis
홈페이지: https://wcleelab.wixsite.com/orgsyn

Highly Sensitive and Selective Mercury Sensor Based on Mismatched Base Pairing with dioxT

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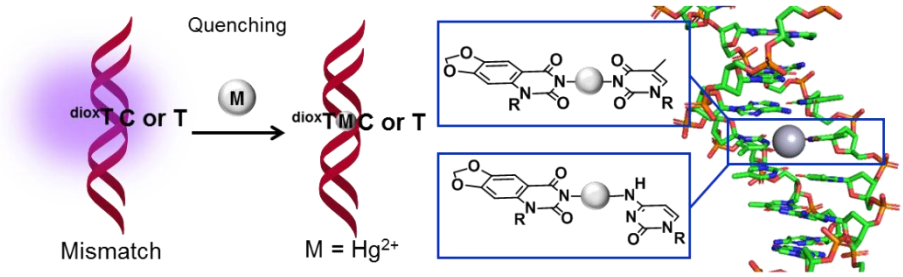
Heavy metal ions are well known for their involvement in important environmental issues, because of their severe effects on human health. In particular, the highly toxic mercury(II) ions are widespread pollutants that arise from industrial waste materials and a variety of natural sources. It is well-known that mercury(II) ions mainly cause several severe health problems, such as kidney failure, brain damage, and heart damage. Since the first report of T-Hg(II)-T binding by Katz and the seminal studies of Ono and coworkers, the knowledge of the binding of mercury ions to T-T mismatched base pairs has led to the rapid development of metal sensors based on DNA. Very recently, we developed new fluorescent thymine analogues based on the dioxoloquinazoline core, ^{dioxT}. ^{dioxT} has desirable biophysical properties as a T surrogate, including complementary base pairing with A.[1] Moreover, ^{dioxT}-containing DNA displays an excellent quantum yield (~0.2) and a remarkable brightness. The notable biophysical and photophysical features of ^{dioxT} instigated us to develop a fluorescent nucleic acid-based metal sensor. Herein, we report the development of a highly sensitive and selective mercury sensor using a new fluorescent nucleobase analogue, ^{dioxT}.[2]



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한지훈

조교수: 안동대학교 화학과(2020~현재)
연구분야: Fluorescent Nucleobase, Nucleic Acid Chemistry, Biophysical Chemistry

Cu-Catalyzed Isocyanation of Benzylic C–H Bonds Enabling High-Throughput Synthesis of Diverse Pharmaceutically Relevant Ureas

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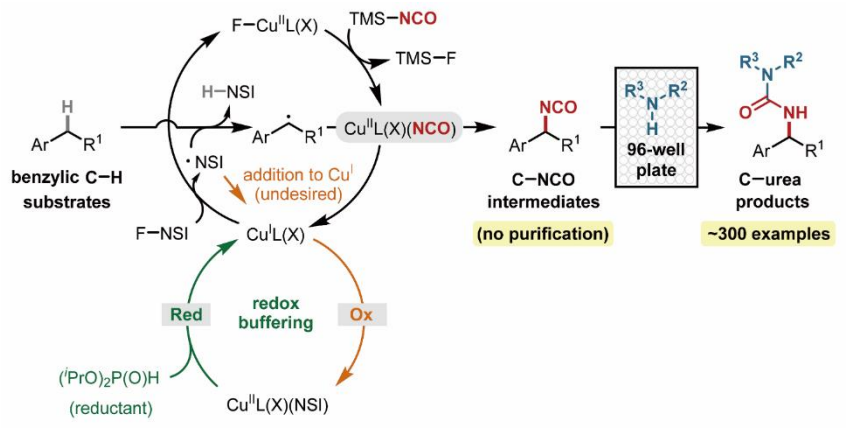
C(sp^3)–H functionalization methods provide an ideal, but still underdeveloped, synthetic platform for medicinal chemistry—harnessing selective functionalization of one specific C–H bond over others in the molecule with an appropriate set of catalysts and reagents remains a huge challenge. We report a Cu-catalyzed method for benzylic C(sp^3)–H isocyanation with TMSNCO as the reagent and *N*-fluorobenzenesulfonimide as the oxidant. This reaction is operationally simple, uses commercially available reagents, and shows high site selectivity with good functional group tolerance. The resulting isocyanate products may be used, without isolation or purification, in a subsequent coupling with primary and secondary amines to afford ureas. This sequential protocol was adapted to the high-throughput synthesis of hundreds of benzylic ureas that exhibit molecular properties compatible with pharmaceutical lead structures.



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서성은

조교수: 아주대학교 화학과(2021~현재)
연구분야: synthetic methodology, bioactive molecule synthesis
홈페이지: https://sites.google.com/view/suhgroup

Cyclic Bis-ammonium Salts as a New Class of Organic Ionic Plastic Crystals (OIPCs)

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Here, we are introducing new type of organic ionic plastic crystals (OIPCs) based on cyclic bis-ammonium cations with various length of alkylene bridges and alkyl side chains. OIPCs usually show long-range order but short-range disorder, typically arising from rotational motions of the molecules, which causes multiple solid-solid transitions and small heat absorption during a melting transition. Before our study, mono-cation based OIPCs have been reported, however we found that symmetric dicationic cyclic ammonium cations with various combinations of different anions also show plastic crystal properties with relatively high melting temperatures. Dicationic imidazolium, pyrrolidinium, piperidinium, pyridinium and ammonium organic cations have been synthesized and their salts with various anions were fully characterized such as spectroscopic structures, thermal properties in stabilities and phase behaviors, and electrochemical properties. All the detail thermal and electrical properties can be controlled by changing the chemical structure of the salts. Possible applications for electrochemical devices have been tried; solid-state electrolytes of dye-sensitized solar cells (DSSCs) and secondary lithium-ion batteries, additives of non-aqueous liquid electrolytes for secondary batteries, and grain boundary/interface modifiers for hybrid Perovskite solar cells.

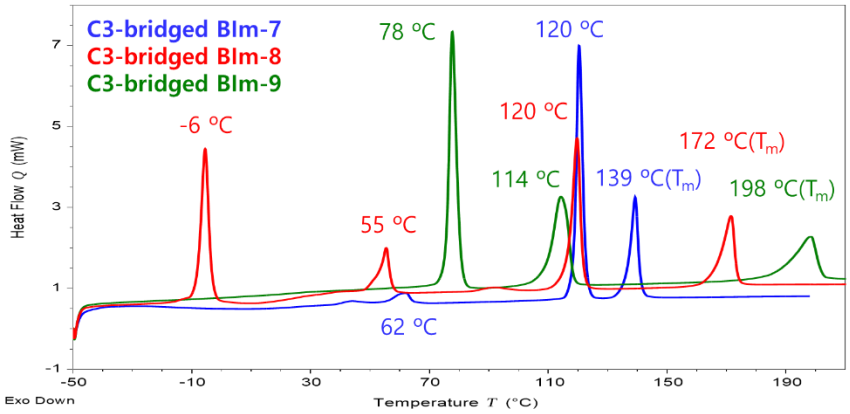

Fig. DSC thermograms of C3-bridged bis-imidazolium PF_6^- salts

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이민재

부교수: 군산대학교 화학과(2013~현재)
연구분야: Organic Ionic Plastic Crystals, Ionic Polymers, Polymer Solid-State Electrolytes, Organic Self-Assembling Materials
https://www.kunsan.ac.kr/chem/index.kunsan?menuCd=DOM_000006902001000000

A Novel Approach for Tuberculosis Chemotherapy Through Disruption of Bacterial Toxin-Antitoxin Systems

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The unique structural feature of the toxin-antitoxin (TA) systems from *Mycobacterium tuberculosis* has inspired scientists to pursue novel antimicrobial agents against tuberculosis, one of the world leading bacterial infections.[1] It has been known that the artificial activation of bacterial toxins by peptide inhibitors can lead to the growth arrest and eventual death of bacterial cells. Optimization of peptides through α-helix stapling method[2,3] based on the structural information of the VapBC TA complex system[4] and in vitro systematic validation led to the discovery of V26-SP-8 and V30-SP-11 stapled peptides.[5] These compounds exhibit enhanced antibacterial activity and cell permeability owing to the stabilizing helical propensity of the peptide, which leads to increased efficacy against multi-drug resistant and extensively drug-resistant tuberculosis. This nascent approach opens a new opportunity toward developing new antibiotic targets for innovative TB therapies.

Acknowledgement

B.J.L. and B.M.K. thank the Kore Drug Development Fund (KDDF-201712-03).

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김병문

조교수, 부교수, 교수: 서울대학교 화학부 (1995~현재)
연구분야: Heterogeneous catalysis, selective organic synthesis, anti-cancer, anti-depression and antibacterial medicinal chemistry
홈페이지: https://yjchoi5715.wixsite.com/synmed

In(III)-Catalyzed Regioselective Syntheses of 1-Naphthaldehydes from 3-Formylchromones

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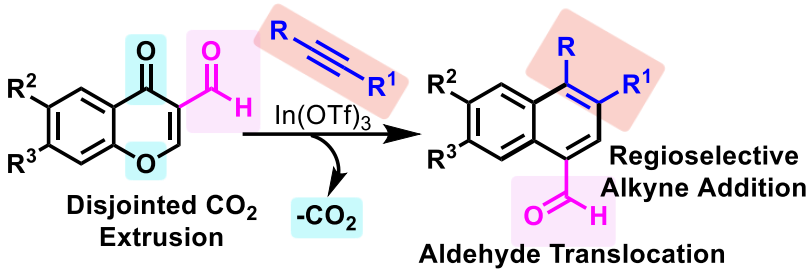
Naphthalenes are important structural elements found in many functional materials, pharmaceuticals, and natural products with numerous applications in academia and industry. They are also widely used as valuable building blocks for the construction of more complex polyaromatics. Conversions of naphthalenes to 1- or 2-naphthaldehydes *via* simple oxidation of alcohols or coupling reaction of functional groups on the naphthalene ring are known. However, direct construction of naphthaldehydes from simple starting materials is rare. The development of an efficient and facile approach to highly functionalized naphthaldehydes from readily available starting materials is still a significant challenge with the potential to greatly broaden access to these privileged building blocks. We have been engaged in the development of novel methodologies for the synthesis of diverse aromatics and heteroaromatics. In continuation of our studies for the development of new methdologies, herein, we describe an In(OTf)3-catalyzed regiocontrolled direct construction of diverse and polyfunctionalized 1-naphthaldehydes through annulation of 3-formylchromones with symmetrical or unsymmetrical alkynes (Scheme 1).



Scheme 1. In(III)-catalyzed regioselective syntheses of 1-naphthaldehydes starting from 3-formylchromones

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이용록

전임강사, 조교수, 부교수, 교수: 영남대학교화학공학부(1995~현재)
연구분야: Synthesis of heteroaromatics and aromatics.
Nanomaterial syntheses and their application
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Asymmetric Oxidative Phenol Coupling to Install Axial Chiral Bonds and Its Application in Chaetoglobin A Synthesis

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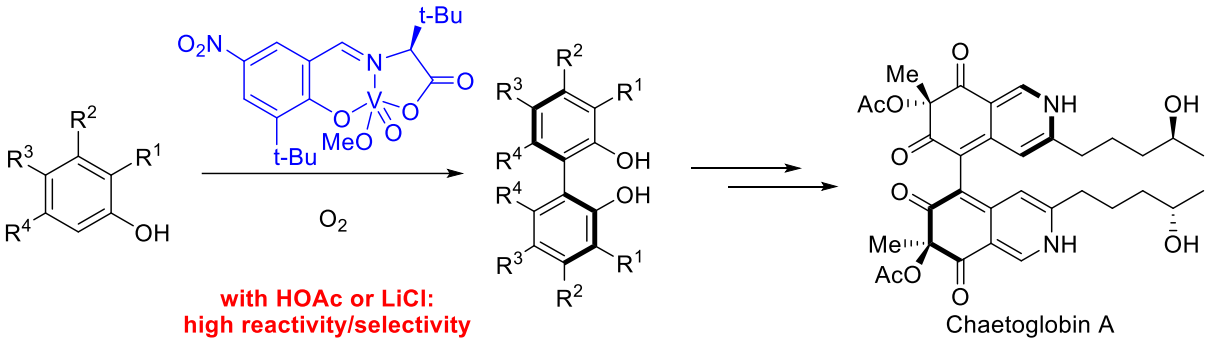

The axial chiral biaryl motif is found in many natural products as well as in structural important in catalysis such as 1,1'-binaphthol. Approaches involving redox-neutral cross couplings, in particular Suzuki couplings, have been successful for a range of binaphthyl and biphenyl structures with some limitations on structure. Over the past 25 years, oxidative asymmetric catalysis has been explored in this context with particular success in the generation of enantioenriched binaphthol structures by means of copper, ruthenium, vanadium, and iron catalysts. The absence of any prefunctionalization at the centers undergoing C–C bond formation confers several advantages to this latter approach with respect to overall efficiency. However, oxidative asymmetric coupling has been noticeably absent with simple phenols vs 2-naphthols. We were inspired to use vanadium complexes as they appear to have the requisite baseline reactivity to catalytically couple phenols. In addition, the success of chiral vanadium catalysts in the asymmetric coupling of naphthols provides support for use of these architectures in the control of atroposelective couplings. To demonstrate a proof of concept, vanadium-catalyzed oxidative phenol coupling enabled the formation of a chiral axis between two identical highly oxygenated bicyclic cores in azaphilone dimer, chaetoglobin A. The first total synthesis of chaetoglobin A was successfully completed in 12 steps from 2,6-dimethoxytoluene.

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강호웅

조교수: 충북대학교 화학교육과(2021~현재)
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Copper-Mediated Oxidative Dehydrosulfurative Carbon-Nitrogen Cross-Coupling of 3,4-Dihydropyrimidine-2-thiones with Amines

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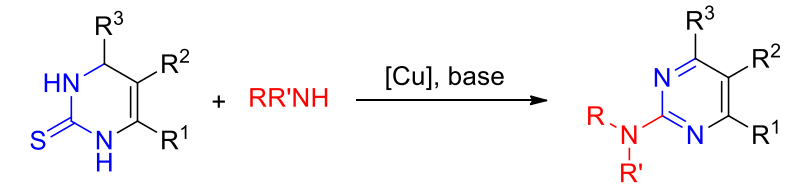
The 2-aryl(alkyl)aminopyrimidine motifs are embedded as a privileged substructure and a key binding fragment toward targets in many important drugs, such as the hypocholesterolemic agent rosuvastatin (Crestor) and the potent anticancer drug imatinib (Gleevec).[1] They have also been proven to trigger the inhibition of protein kinases or receptors in many development candidates.[2] Despite their biological importance, the synthetic strategy towards these compounds is limited in scope and generality, especially for the rapid generation of a diverse range of such compounds. Usually, the fully substituted 2-aryl(akyl)aminopyrimidines are obtained by nucleophilic aromatic substitution or metal-catalyzed carbon-nitrogen cross-coupling of C2-(pseudo)halopyrimidines with amines, most of which require synthesis of pyrimidine partners in multiple steps.[3] Herein, we report one-step synthesis of 2-aryl(alkyl)aminopyrimidines from 3,4-dihydropyrimidin-1*H*-2-thiones (DHPMs) via copper-mediated dehydrosulfurative C-N cross-coupling and concomitant oxidative dehydrogenation. The results demonstrate that the thiono group is a suitable leaving group of the carbon in the copper-mediated carbon-nitrogen cross-coupling reactions.[4]



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손정훈

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연구원: 한국파스퇴르연구소(2007~2011)
차장: LG생명과학(2005~2006)
연구분야: Synthesis of heterocyclic compounds, metal-catalyzed chemoselective coupling using FRET-based method
홈페이지: https://chem.cnu.ac.kr/chem/

Supramolecular Chemistry for Biofunctional Materials

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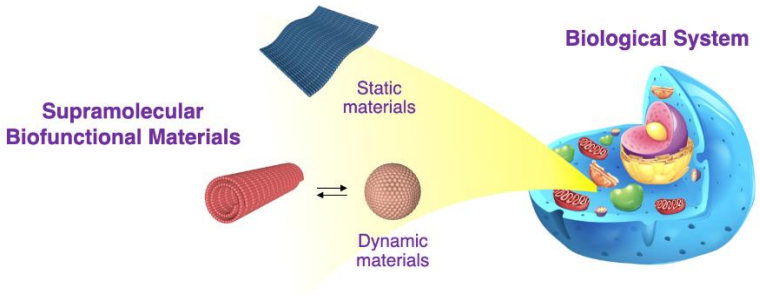
Various biological systems rely on the supramolecular assembly of biomolecules through noncovalent bonds for performing sophisticated functions. Among diverse self-assembling modules, aromatic amphiphiles can serve as remarkable candidates for the creation of well-defined supramolecular structures owing to their rigidity and the π–π stacking of aromatic groups. I present the switchable assembly for biofunctional materials via supramolecular chemistry principles. For example, dynamic tubular pores undergo rapid switching between open and closed states in response to a thermal signal in water. Notably, this pore switching mediates a controlled water-pumping catalytic action for the dehydration reaction. A virus-like hierarchical assembly with the native DNA and a synthetic coat shows repeated collective helicity switching triggered by pH change. This collective helicity inversion occurs during translocation of the DNA–coat assembly into intracellular compartments. Translating DNA conformational dynamics into a higher level of hierarchical dynamics may provide an approach to create DNA-based nanomachine. Homochiral porous nanosheets are presented with open-closed pore switching. The porous 2D structures can serve as enantiomer sieving membranes which exclusively capture a single enantiomer in a racemic mixture solution with high uptake capacity. The entrapped guests inside the pores can be pumped out by pore closing triggered by salt. Moreover, I present supramolecular concepts to translate the adaptive nature of biological systems into synthetic self-assembly.



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김용주

부교수: 고려대학교 KU-KIST융합대학원 & 융합에너지공학과 (2019~현재)
연구분야: Supramolecular Chemistry, Nanomedicine, Bioactive Materials
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Functional Fluorescent Probes for Image-guided Surgery of Human Glioblastoma

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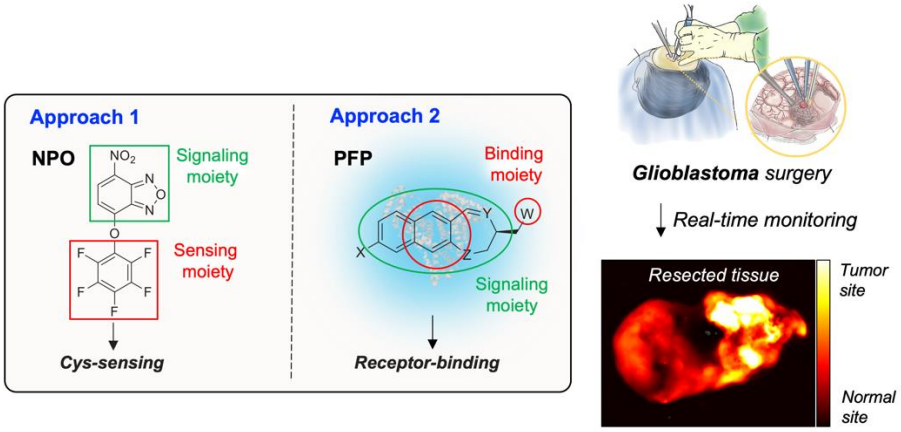
Development of the real-time monitoring methods of pathological features in clinical tumor surgery is in the spotlight for accurate resection for the targeted disease site. Typical methods such as polymerase chain reaction, western blot, and immunofluorescence are not utilized in an operating room, but fluorescence-based imaging-guided surgery (FGS) using fluorescence materials have merit in terms of field usability. Recently, we have focused on developing functional fluorescent probes for image-guided surgery of human glioblastoma (GBM), which is the most aggressive type of cancer that begins within the brain. We have two different approaches as below, and we believe that both approaches for visualization of GBM would have high potential and propose the future road of the fluorescent probe in the real-time FGS.

Approach 1 (reaction-based sensing): We developed a functional fluorescent probe (named **NPO**) for the detection of the cysteine (GBM-metabolite) levels in human-derived GBM cells, GBM-xenograft models, and human biopsy samples [1]. The probe consists of a pentafluorophenol (sensing moiety) and nitrobenzoxadiazole (fluorophore), and it showed high selectivity, sensitivity, and biocompatibility.

Approach 2 (binding-based sensing): We developed a functional protein-fluorophore-peptide complex (named **PFP**) for the selective visualization of the GBM site. The **PFP** performed GBM cell-targeted imaging and visualization of on-site GBM biopsy derived from the patient [2].



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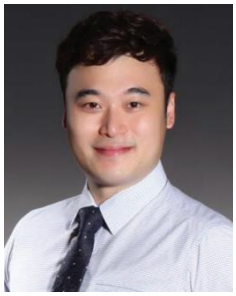

김도경

조교수: 경희대학교 의과대학 의예과 (2017~현재)
연구분야: fluorescent materials, hybrid nano-materials, nanotherapeutics
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Group 10 Transition Metal (Ni, Pd)-Catalyzed Asymmetric Hydro-functionalization of Alkenes

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Alkenes have been regarded as attractive starting materials in modern organic syntheses owing to the abundance, readily availability, and synthetic versatility of these substrates. Among the transformation of alkenes, hydrofunctionalization, an addition of a hydrogen and a functional group across a carbon-carbon double bond, is arguably one of the most efficient methods to prepare more complex molecules from simple alkenes. As a result, a diversity of approaches have been developed. Among these strategies, metal-hydride catalyzed olefin hydrofunctionalization has been received particular attention owing to the fact that asymmetric transformations can be achieved by suitable choice of catalyst/ligand system.

In this talk, I will present our group's effort on the development of asymmetric hydrofunctionalization of olefins (vinylarenes) enabled by novel nickel- or palladium-hydride based catalytic system. In detail, preliminary results on the palladaelectro-catalyzed hydroalkoxylation of vinylarenes will be presented. Initial results on nickel-hydride catalyzed hydroacylation and hydroarylation of styrenes will also be discussed.

신광민

조교수: 성균관대학교 화학과(2020~현재)
연구분야: transition metal-catalysis, asymmetric catalysis, ligand design
홈페이지: https://shinkw34.wixsite.com/kmshinlab

An Abiotic Fluorescent Probe for the Detection and Quantification of Carcinoembryonic Antigen

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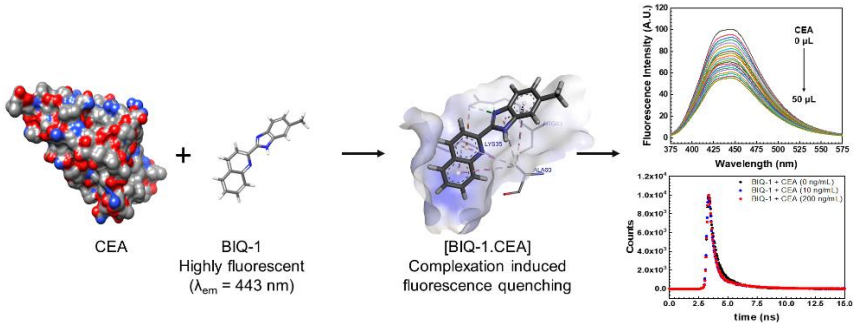
Detection of cancer biomarkers in serum is the hallmark for the development of molecular diagnostics. The detection of blood-based biomarkers such as carcinoembryonic antigen (CEA) allows identifying cancer patients from the general population. The CEA serum levels are low (2.5 - 3.0 ng mL−1) in healthy individuals than in patients (> 3.0 ng mL−1) with several types of cancers, including colorectal carcinoma, colon adenocarcinoma, lung cancer, breast cancer, and gastric cancer. A variety of methods, including ELISAs, colorimetric assay, fluorescence assays, surface-enhanced Raman scattering (SERS), and DNA chips, exist to detect CEA. The common disadvantages of these methods include requisite incubation time, the requirement of highly trained professionals, and expensive instrumentation. On the contrary, the ratiometric fluorescence method is advantageous because it is ultra-fast, easy-to-operate, real-time, and low-cost. Therefore, an abiotic, highly-specific fluorescent probe would obviate the current immunoassay-based methods in favor of an abiotic, highly-specific fluorescent probe. Herein, an abiotic fluorescent probe, **BIQ-1**, was conceived using bioinformatics tools and molecular docking techniques for the rapid yet straightforward detection of CEA in a buffer matrix resembling serum. In a simple cuvette-based experiment, **BIQ-1** exhibited LoD of 3.04 ng/mL for CEA in the clinically significant region (0~200ng/mL). The BIQ-1 did no show considerable interference from the possible interfering components such as hemoglobin, intralipid, and HSA in several-fold higher concentrations (μg/mL) than CEA.



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Satish Balasaheb Nimse

조교수: 한림대학교 화학과
연구분야: Biomarker detection, imaging and sensing, Denovo drug design and drug discovery
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Investigation of Regioselective C–H Functionalization of Heteroarene

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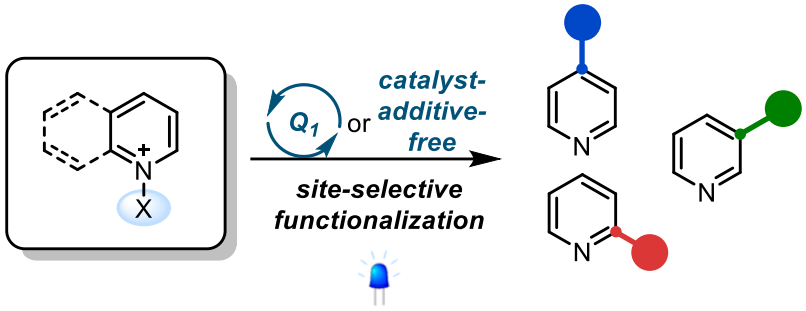
The site-selective C–H bond functionalization of heteroarenes is highly desirable in the broad field of chemical research. Chemical methods to achieve this goal could have broad application potential in synthetic organic chemistry, considering the reduction in the number of synthetic steps and the abundance of inexpensive starting materials. The new catalytic synthetic methods allow us to perform the unprecedented disconnection of target molecules, affording innovative and imaginative synthetic strategies of so-called “privileged scaffolds”. Visible-light-induced site-selective heteroarylation of remote C(sp^3)–H bonds has been accomplished through the design of a photoexcited quinolinone catalyst (Q_1). The synthetic potential of pyridinium salts has been demonstrated as versatile pyridine surrogates to address various chemical transformations.6 In light of these benefits, our group leveraged the steric and electronic properties of the N-substituent of pyridinium salts to control the functionalization of pyridines. These new catalytic synthetic methods will function as competent tools directly utilized in cross-coupling reactions capable of connecting privileged building blocks, providing opportunities for the successful implementation of fragment-based drug design (FBDD) and eventually streamline drug discovery research.



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홍승우

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연구분야: development of new reactions & catalysis, medicinal chemistry & Chemical Biology
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Interplay among Conformation, Intramolecular Hydrogen Bonds, and Chameleonicity in the Membrane Permeability and Cyclophilin A Binding of Macrocyclic Peptide Cyclosporin O Derivatives

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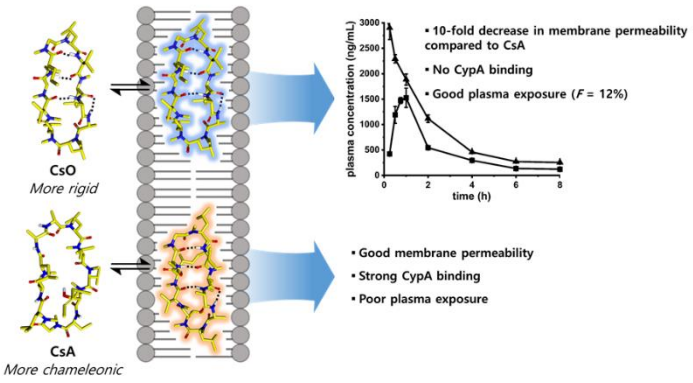
A macrocyclic peptide scaffold with well-established structure-property relationship (SPR) is desirable to tackle the "undruggable" targets. Here, we adopted a natural macrocycle, cyclosporin O (**CsO**) and its derivatives (**CP1**–**3**), and evaluated the impact of conformation on membrane permeability, cyclophilin A (CypA) binding, and the pharmacokinetic (PK) profile. Compared to cyclosporin A (**CsA**), a well-known chameleonic macrocycle, **CsO** showed a similar conformation in a nonpolar media but less chameleonic behavior in a polar environment. The weak chameleonicity of **CsO** resulted in decreased membrane permeability; however, the more rigid conformation of **CsO** was not detrimental to its PK profile. **CsO** exhibited a higher plasma concentration than **CsA**, which resulted from minimal CypA binding and lower accumulation in red blood cells, and moderate oral bioavailability (F = 12%). Our study helps in the understanding of **CsO**, a macrocyclic peptide less explored than **CsA** but with more potential for diversity generation and rational design.



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서지원

조교수, 부교수 GIST 화학과(2010~현재)
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Fascinating Construction and Restructure of N-Heterocyclic Compounds

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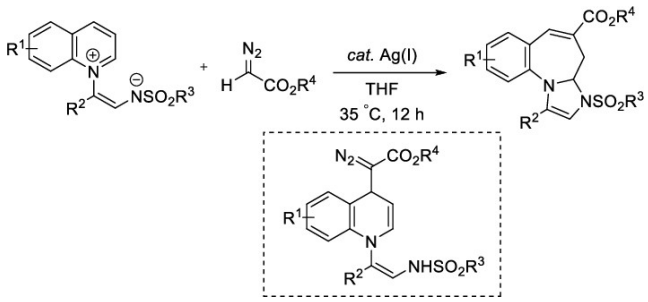
Heterocyclic compounds found in numerous natural products are an important class of structural motifs. Their potent biological activities and interesting medicinal effects have an impact on the pharmaceutical industry. [m+n] dipolar cycloaddition is a powerful and widely used strategy as it ensures 100% atom economy with a single operation. Our group developed unprecedented N-aromatic zwitterions, which are quite stable and exhibits different pattern of charge distribution in comparison with that of typical dipoles, to serve a five-atom synthon for [5+n] cycloaddition reactions. Surprisingly, developed zwitterion could be employed as a reaction site-switchable reactant depending on the reacting partners; it could act as 2π-dipolarophiles for the [m+2] cycloaddition reactions as well.

Along with cycloadditions, the restructuring of ring skeletons, such as contraction, expansion, deconstruction, and fusion, is also an efficient and prevalent method to achieve molecular diversity. In this seminar, we will discuss the construction and restructure of N-heterocyclic compounds using atypical N-aromatic zwitterions. First, a catalytic ring-expansion of N-aromatic zwitterions through 1,4-dearomative addition of diazoacetates will be presented for the construction of various fused azepines. Next, an unprecedented strategy for the cycloadditive ring-contraction affording multi-substituted pyrrolo[1,2-a]quinolines will be briefly introduced.



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유은정

조교수, 부교수: 경희대학교 응용화학과(2018~현재)
조교수: 강원대학교 화학과(2012~2018)
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Cu-Catalyzed Hydroalumination of Allenes with DIBAL-H: Synthesis of α-Quaternary Carbon Centers

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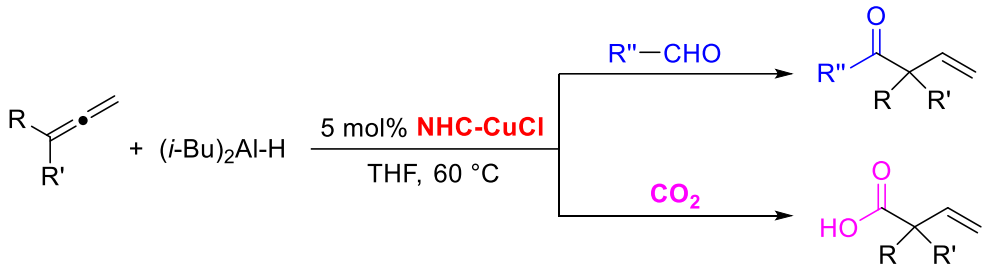
Copper-catalyzed hydrometalation of allenes with a hydride source is an attractive method for preparing allylic metal reagents because it is a simple and atom economical process, uses an inexpensive and easy to handle copper catalyst and uses readily available allene substrates. In recent studies, a few examples of copper hydride-catalyzed reactions with allenes have been reported. However, only silane has been used as a hydride source, resulting in the generation of allylcopper intermediates via hydrocupration of a copper hydride complex with allenes. In this presentation, we describe a new approach to allylaluminum reagents through Cu-catalyzed hydride addition of diisobutylaluminum hydride (DIBAL-H) to allenes and applications for developing unexplored allylation reactions by applying the intrinsic reactivity and Lewis acidity of aluminum. An *N*-heterocyclic carbene (NHC)-based copper complex played an important role in promoting hydride addition of DIBAL-H to various functionalized allenes and controlling its regioselectivity. This catalytic reaction was applied to synthesis of allylic ketones with α-tertiary and α-quaternary centers through tandem addition of allylaluminums to aldehydes/Oppenauer oxidation. In addition, in situ generated allylaluminums were used for carboxylation with carbon dioxide, affording carboxylic acids with α-quaternary carbon centers.



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이윤미

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Development of Versatile Initiator Films for Surface-Initiated Polymerization

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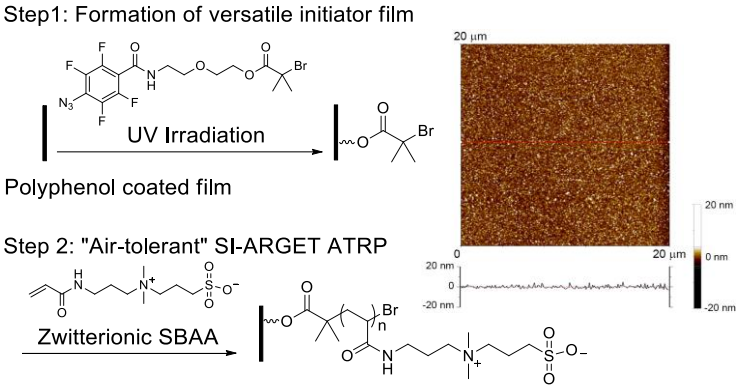
In this study, we developed a versatile initiator film that can form functional brush by surface-initiated polymerization (SIP). Initially, polyphenolic compounds were coated on various surfaces, including gold, titanium oxide, stainless steel, glass, and indium tin oxide, followed by covalent functionalization with an aryl azide-based initiator under photo-irradiation. The resultant initiator film was formed under mild coating conditions and fulfilled uniformity and transparency.[1] In particular, combination with a photolithographic technique allowed the immobilization of initiators only on the intended region.[2] Subsequently, developed initiator films can be further utilized to form an antifouling brush by proceeding with SIP using sulfobetaine acrylamide (SBAA). Instead of typical, atom transfer radical polymerization (ATRP) technique which require air-free conditions, we utilized an activator regenerated by electron transfer (ARGET) ATRP under air conditions without performing deoxygenation step.[3] Overall, our developed initiator layer act as a surface platform to grow poly(SBAA) brush on various surfaces, and enabled their pattern generation.



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홍대화

조교수: 부산대학교 화학과(2017~2021)
부교수: 부산대학교 화학과(2021~현재)
연구분야: Functional organic materials, surface coating, polymer science
홈페이지: https://dwhong.wixsite.com/dwhong

Water-Driven Biomimetic Catalytic Enantioselective Protonation

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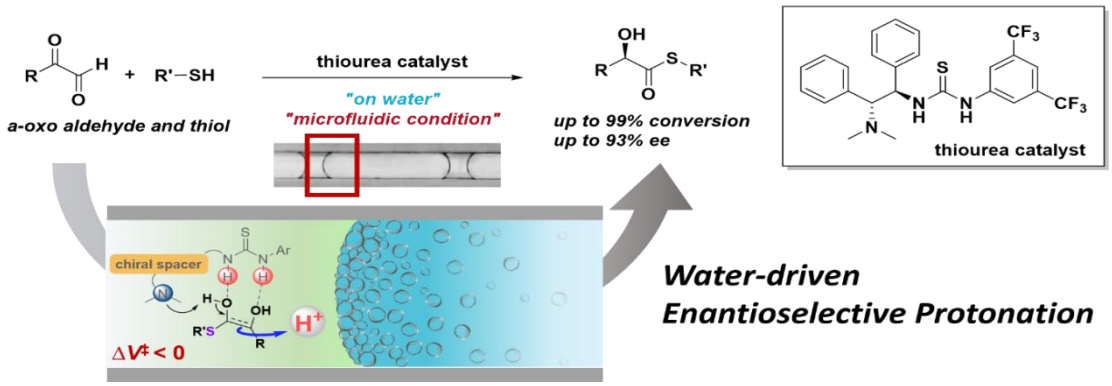
Catalytic enantioselective protonation of a prochiral carbanion in water is a common transformation in biological systems, but has been beyond the capability of synthetic chemists since unusually rapid movement (1−2 ps) of a proton in water leads to uncontrolled racemic protonation. Therefore, governing the movement of a proton in water within a catalytic cycle in an enantioselective manner is an extremely challenging task. In this workshop, we present a successful example of bio-inspired enantioselective protonation in water, revealing how to govern the movement of a highly mobile proton in water in an enantioselective manner.[1] Water enables a highly enantioselective glyoxalase I-mimic catalytic isomerization[2] of hemithioacetals which proceeds via enantioselective protonation of an ene-diol intermediate. The use of on-water condition turns on this otherwise extremely unreactive catalytic reaction as a result of the strengthened hydrogen bonds of water molecules near the hydrophobic reaction mixture. Furthermore, under on-water conditions, especially under biphasic microfluidic on-water conditions, access of bulk water into the enantio-determining transition state is efficiently blocked, consequently enabling the enantioselective introduction of a highly ungovernable proton to a transient enediol intermediate, which mimics the action of enzymes. We believe that our results may provide a potential starting point for designing more challenging biomimetic catalytic asymmetric reactions in which water helps regulate reaction rates and selectivity.



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송충의

문행석좌교수: 성균관대학교 화학과 (2020~현재)
연구분야: asymmetric organocatalysis, biomimetic catalysis, prebiotic chemistry, specifically, the origin of homochirality (chirality amplification process)

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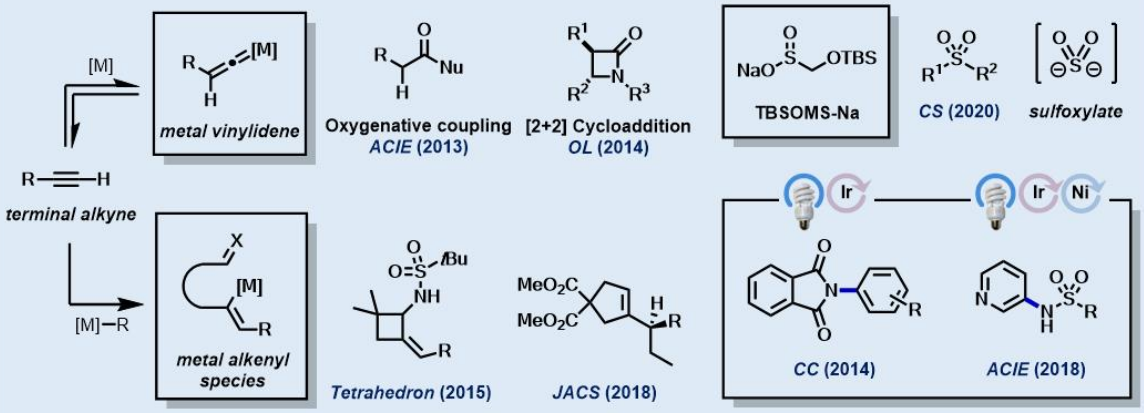
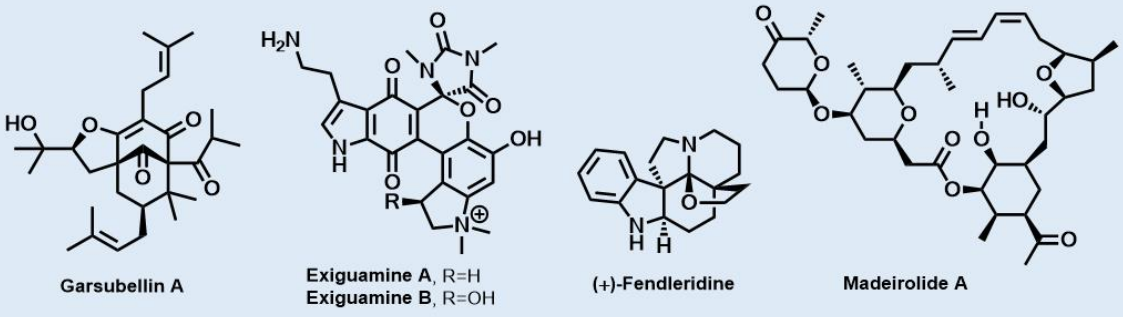
촉매 반응 개발



천연물 전합성

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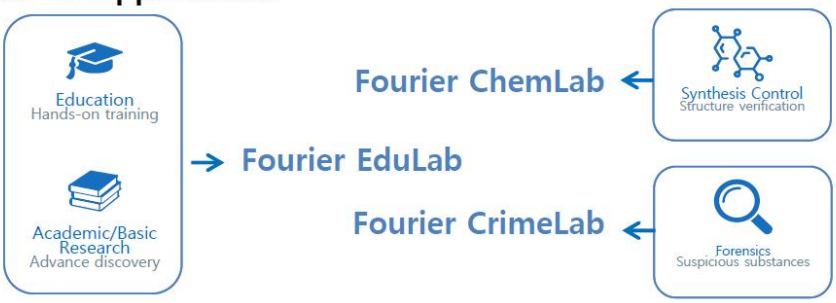

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타　　입 : 듀얼 채널
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최대 압력 : 1.0Mpa(145psi, 10bar)
검 출 기 : 듀얼파장·싱글파장 선택 가능
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옵　　션 : ELSD, RI, TLC Image Reader

싱글

모 델 명 : AI-580S
타　　입 : 싱글 채널
한 번에 한 개 샘플 분리 정제 가능
펌프 유량 : 최대 80ml/min
최대 압력 : 1.0Mpa(145psi, 10bar)
검 출 기 : 듀얼파장·싱글파장 선택 가능
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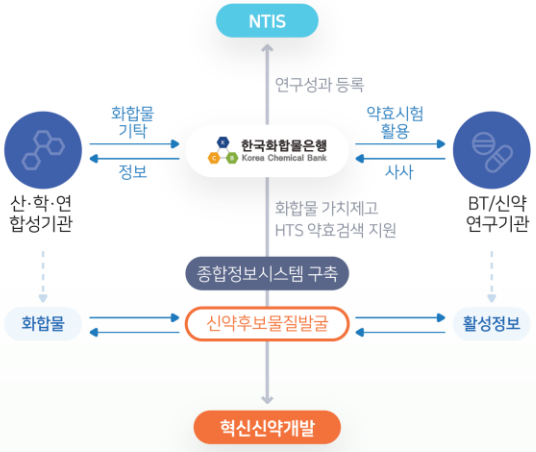

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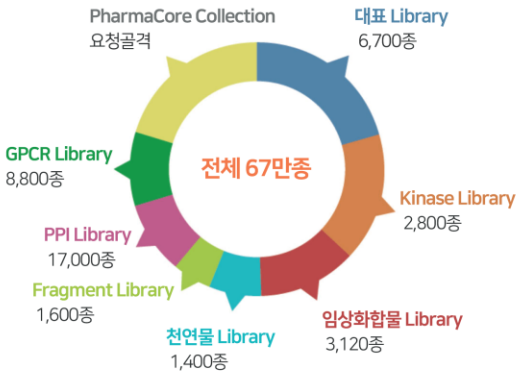

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