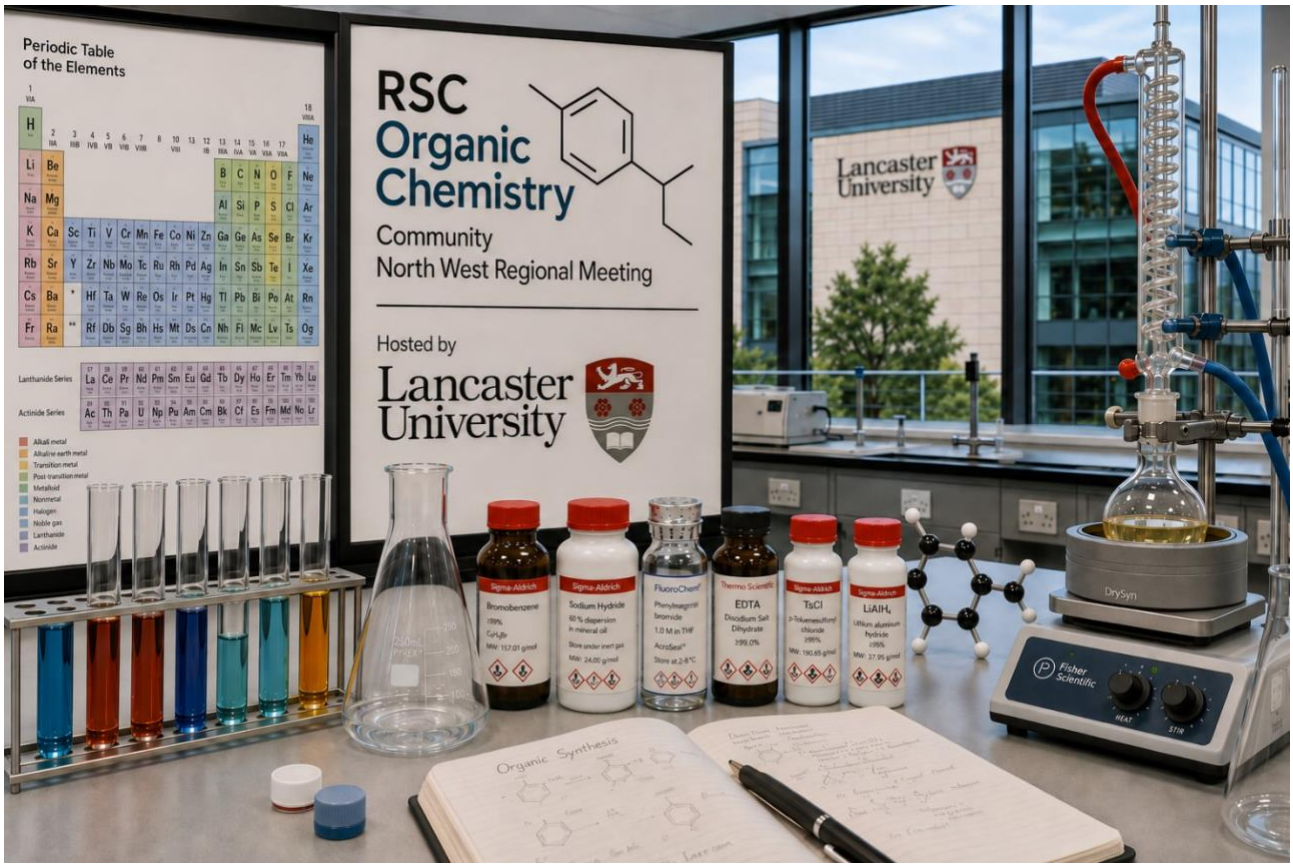
RSC Organic Chemistry Community North West Regional Meeting 2026

3rd July 2026

Lancaster University



AI generated image – *can you spot everything in the image that does not represent Chemistry accurately?*

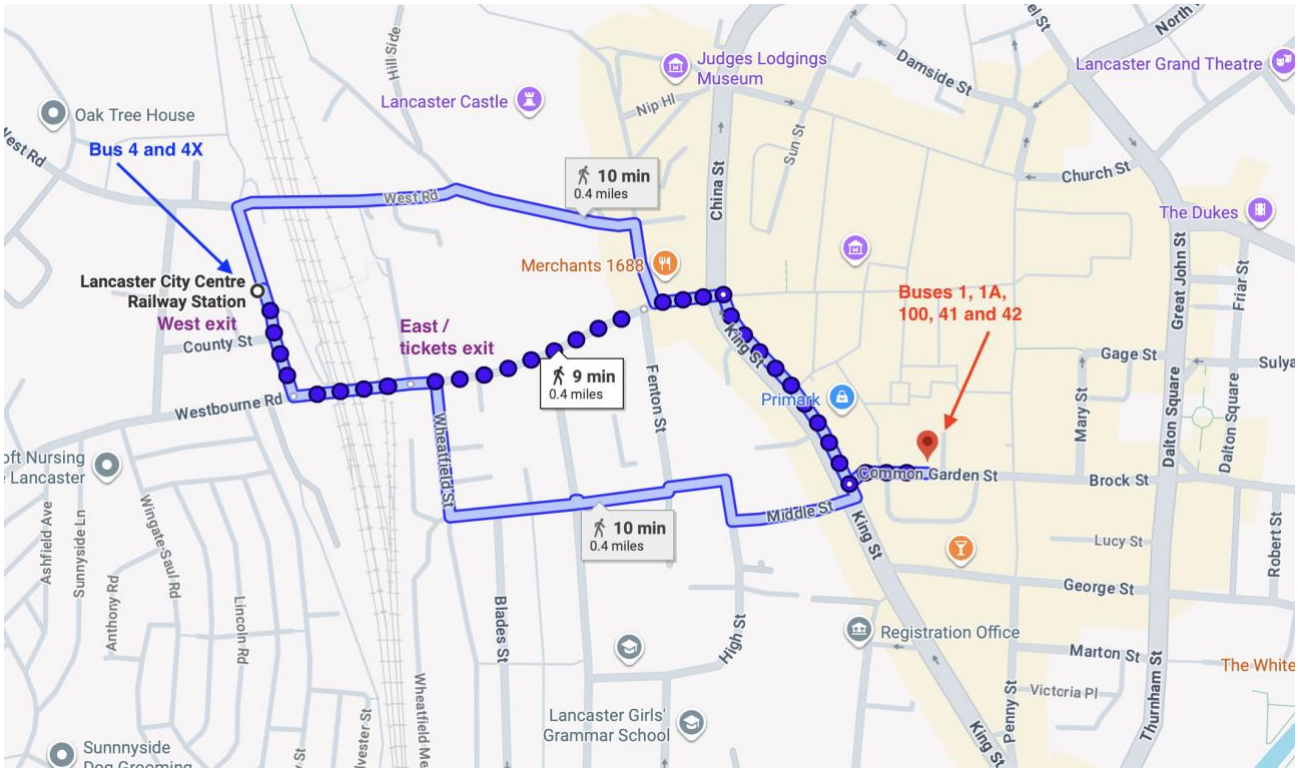
Contents

List of Sponsors and Exhibitors

A range of exhibitions from the below can be found in County South LT.

Where to Find Us

The 4 and 4X bus services operate between Lancaster Railway Station (Platform 3 exit) and Lancaster University every hour Monday to Friday daytimes. The journey time is around 25 minutes. Multiple other more frequent services (1, 1A, 100, 41, 42) go to the University from Common Garden Street, a 9 minute walk from the station.
Taxis are available at the station (West exit), but it can be advisable to book in advance (these will pick you up at the East / ticket office exit). Reliable Lancaster taxi operators are 848 taxis (01524 848848), or 32090 taxis (01524 32090).

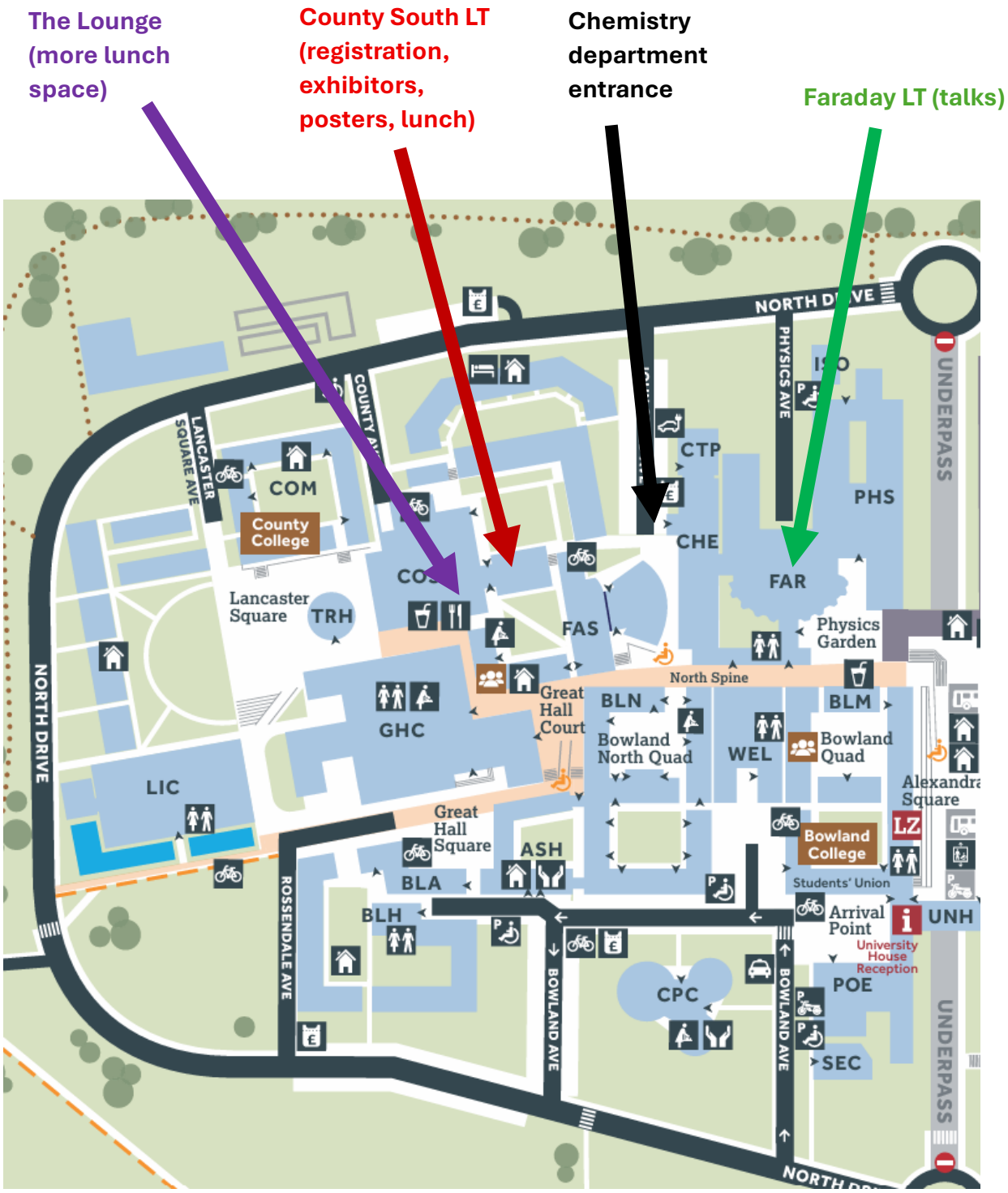


If you choose to drive, the postcode for Chemistry Department is LA1 4YB. There are over 750 visitor parking spaces across visitor car parks A to M and South West Campus, with ANPR cameras in effect across the campus. The charge is £6.20 for the day. The closest visitor parking to the Chemistry building is car parks B and C.

RingGo Cashless Parking Solution is available across all visitor car parks, as well as at the Sports Centre, Health Innovation Campus, and South West Campus. Visitors can pay for their parking by the RingGo app or using the RingGo website. Detailed instructions on using RingGo to pay for parking are signposted at all visitor car parks.

Blue Badge holders are exempt from all parking charges and can park in dedicated accessible parking bays in all parking zones. Please contact the Car Parking team by emailing car-parking@lancaster.ac.uk to pre-arrange accessible parking with a Blue Badge.

Registration in the morning is at County South Lecture Theatre, which can be located following the signs around the campus. A detailed campus map can be found on [the Lancaster University webpage], and at the end of this booklet, with an excerpt shown below.



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Scientific Programme

Registration from 9:00 ***with breakfast and exhibitors*** (County South LT).

Session 1 (Faraday LT) ***Chair: Dr Nick Evans***

10:15–10:30 Welcoming remarks and housekeeping

10:30–11:00 Dr Julien Doulcet (Lancaster University). "*Harnessing Amine Feedstocks for C(sp^3)–C(sp^3) Bond Formation via Radical Cross-Coupling*"

11:00–11:30 Dr Aaron Trowbridge (University of Manchester). "*Biomimetic N-terminal homologation of amino acids"*

11:30–12:00 Dr John Ward (University of Liverpool). "*Discovery of Anthraquinone-Based Photocatalysts for Decarboxylative Giese Reactions*"

12:10–13:50 ***Lunch, Exhibitions and Poster Session*** (County South LT and The Lounge)

Session 2 (Faraday LT) ***Chair: Dr Jonathan Ward***

14:00–14:30 Dr Jamie Docherty (Lancaster University). "*Synthetic Innovation in Strained Heterocycles and DNA-Encoded Libraries"*

14:30–15:00 Dr Andrew Lewis (Manchester Metropolitan University). "*Covalent Chemistry and Computational Discovery: Integrating Chemical Biology and AI to Probe Mechanisms of Disease*"

15:00–15:30 Dr Jean-Marc Henry (Astra Zeneca). "*Development and implementation at 200kg scale of a transamination process*"

Session 3 (Faraday LT) ***Chair: Dr M. Paz Muñoz***

15:30–16:30 Plenary Lecture: Prof Donna Blackmond (Scripps Research & University of Liverpool). "*Mechanistic Understanding of Complex Catalytic Reactions Through a Temperature Scanning Protocol"*.

16:30-16:40 Presentation of the 2025 Centenary Prize for Chemistry and Communication medal to Prof Donna Blackmond by M. Paz Muñoz (RSC OCC).

16:40 Concluding remarks and poster prizes (sponsored by RSC OCC & RSC Lancashire local section, CEM and Shimadzu)

17:00-18:00 ***Drinks reception*** (County South LT).

Oral Presentations

Harnessing Amine Feedstocks for C(sp³)–C(sp³) Bond Formation via Radical Cross-Coupling

Kevin Bucher, Julien Doulcet[1]

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Abstract: Amines are ubiquitous motifs in naturally occurring compounds and pharmaceuticals and, as abundant feedstocks, are widely used as building blocks in chemical synthesis. While amines have traditionally been exploited for C–N bond formation, their use as precursors for C–C bond construction is attracting increasing attention.[1] In this context, bimolecular homolytic substitution (S_H2) has recently emerged as a powerful strategy for C(sp^3)–C(sp^3) bond formation, enabling the selective cross-coupling of two transient radicals.[2] This approach is particularly attractive because such bonds remain challenging to access using conventional cross-coupling methods and because S_H2 enables the construction of quaternary carbon centres, a highly desirable feature in modern drug discovery.

This talk will describe our efforts to develop a strategy for the selective cross-coupling of two radical species, from initial conceptual design to its successful realisation in the hydrofunctionalisation of alkenes using amine-derived redox-active pyridinium salts (**2**).[3] The transformation developed in our laboratory represents the first use of redox-active pyridinium salts in an S_H2-mediated process and employs a single iron–porphyrin catalyst to mediate three key steps: generation of a secondary or tertiary radical from an alkene through metal-hydride hydrogen atom transfer (MHAT), reduction of the redox-active pyridinium salt, and C–C bond formation through S_H2. A broad range of alkenes (including α-heteroatom-substituted substrates bearing N, O, S, B and Si substituents) provide the corresponding hydrobenzylation products **3** in good to high yields (Fig. 1). The method is further demonstrated through late stage functionalisation of drug molecules, highlighting its synthetic utility.

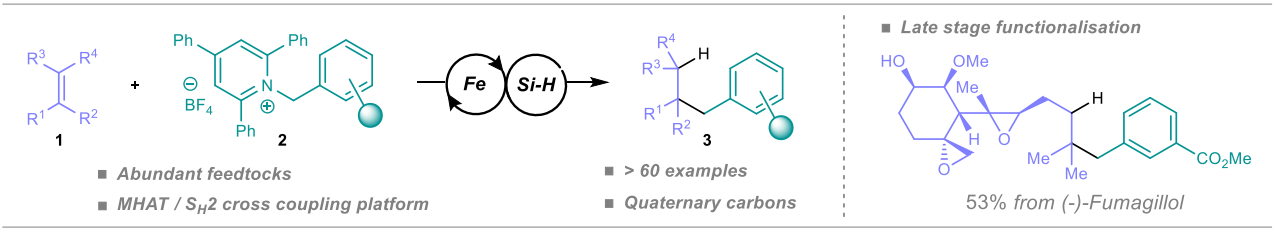

Fig. 1 Deaminative radical mediated C(sp^3)-C(sp^3) cross-coupling

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2 (a) Y. Zhang, K.-D. Li and H.-M. Huang, *ChemCatChem*, 2024, **16**, e202400955; (b) I. M. McWhinnie, R. T. Martin, J. Xie, R. Chen, C. N. Prieto Kullmer and D. W. C. MacMillan, *J. Am. Chem. Soc.*, 2025, **147**, 23351–23366.

3 K. Bucher and J. Doulcet, manuscript in preparation.

Biomimetic N-terminal homologation of amino acids

Andre Bossonnet, Ben Hillman, Cristina Trujillo, Aaron D. Trowbridge
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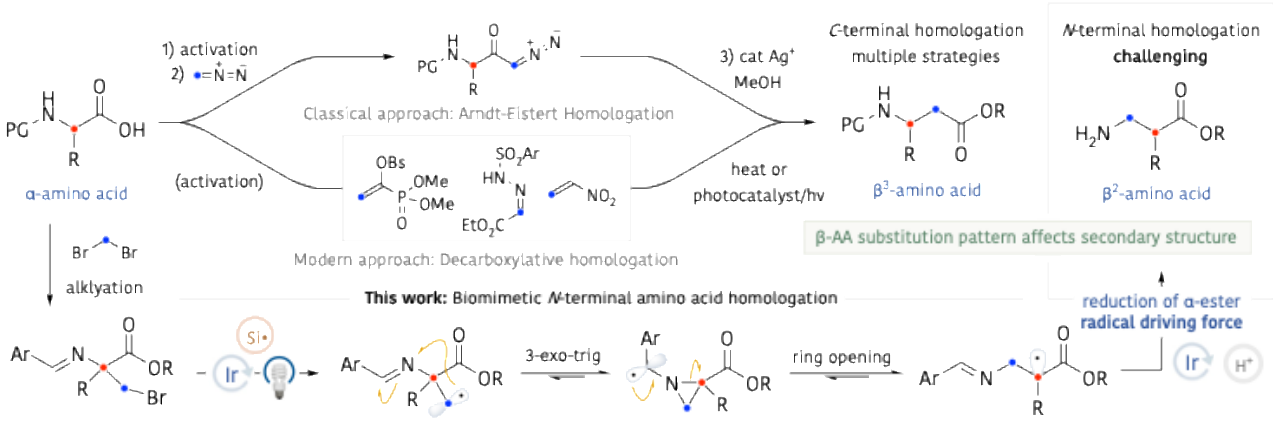
Abstract: One-carbon homologation is a key tactic used in the lead optimization of small-molecule pharmaceuticals due to the impact such modifications can have on target affinity and physicochemical properties. Within this arena, homologated amino acids, β-amino acids, are particularly appealing building blocks due to their improved resistance to proteolysis and conformational and dynamic properties, which can be precisely controlled through the position of the side chain. However, while many elegant homologation strategies have been developed for the synthesis of β^3-amino acids via decarboxylation, preparation of β^2-amino acid homologues remains underexplored. We have developed a general biomimetic strategy for the *N*-terminal homologation of amino acids using photoredox catalysis. Key to the success of this approach is a radical translocation cascade driven by singlet-electron transfer. This methodology provides streamlined access to a range of cyclic and acyclic β^2-amino acids and phosphonates, providing new synthetic opportunities within drug discovery programs.[1]

Fig. 1 Strategy for biomimetic *N*-terminal homologation of amino acids using photoredox catalysis



References

1 *Manuscript in submission*

Discovery of Anthraquinone-Based Photocatalysts for Decarboxylative Giese Reactions

Daniel Anning,[1] Omer Omar, [1] Adrian Gardner, [1] Martin Cattoen,[2] Alessandro Troisi, [1] John W. Ward[1]
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Abstract: Photoredox catalysis is dominated by transition-metal complexes, which offer excellent performance but are costly, scarce, and environmentally unsustainable.[1] The development of efficient organic photocatalysts is therefore an important challenge. High-throughput virtual screening (HTVS) provides a promising route to accelerate catalyst discovery by enabling the rapid evaluation of large chemical spaces.[2] In this work, we employed a previously developed HTVS workflow to identify new organic photocatalysts for the decarboxylative 1,4-radical conjugate addition (Giese) reaction.[3] Computational screening generated a shortlist of 316 candidates, from which 1,4-bis(acetamido)anthraquinone (1,4-AAAQ) emerged as an active photocatalyst. Studying the effect of amide substitution on the anthraquinone core led to the identification of 1,6-bis(acetamido)anthraquinone (1,6-AAAQ), which proved to be a relatively general photocatalyst, delivering moderate to high isolated yields across a range of carboxylic acid substrates. To understand the origin of this enhanced activity, mechanistic studies were conducted using transient absorption spectroscopy to probe the excited-state dynamics of the photocatalysts. By integrating these mechanistic insights with computational screening, we aim to establish structure–property relationships that can guide future HTVS campaigns and accelerate the discovery of sustainable organic photocatalysts.

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2 Ö. H. Omar, M. del Cueto, T. Nematiaram, A. Troisi, *J. Mater. Chem. C*, 2021, **9**, 13557-13583
3 D. M. Kitcatt, S. Nicolleb and A-L. Lee, *Chem. Soc. Rev.,* 2022, **51**, 1415-1453

Synthetic Innovation in Strained Heterocycles and DNA-Encoded Libraries

Jamie H. Docherty
Department of Chemistry, Lancaster University, Lancaster, LA1 4YB, United Kingdom
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Abstract: Discovery chemistry does not need bigger libraries of familiar molecules. It needs innovative chemistry that breaks into molecular space we still cannot reach. Strained heterocycles offer one route into that territory. Selective [4π]-photocyclisation of pyridones gives access to Dewar pyridones: compact, highly strained, heteroatom-rich scaffolds that are difficult to obtain by conventional synthesis, but highly attractive as bioisosteric replacements and versatile platforms for downstream diversification. The same imperative applies in DNA-encoded library synthesis, where the chemistry used to build screening collections still lags well behind the structural ambition of modern drug discovery. Current libraries remain heavily biased toward synthetically convenient, low-complexity molecules, and expanding their value demands DNA-compatible reactions that deliver improved three-dimensionality. By developing *on-DNA* cycloaddition chemistry and related transformations, new routes are opening to C(sp^3)-rich, structurally interesting motifs that are largely absent from existing DEL collections. The core tenet is simple: advances in discovery will not come from making more of the familiar, but from finally learning how to access new chemical space.

Fig. 1. Innovation in the synthesis of novel building blocks and development of *on-DNA* synthetic chemistry for DNA-encoded libraries.

Covalent Chemistry and Computational Discovery: Integrating Chemical Biology and AI to Probe Mechanisms of Disease

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Abstract: Artificial intelligence (AI) and machine learning (ML) are increasingly influencing chemical biology and drug discovery by enabling new approaches to target identification and molecular design. These methods provide valuable guidance for the development of chemical tools to interrogate and modulate biologically relevant proteins. In parallel, covalent chemistry has re-emerged as an important modality, supporting the development of potent and selective therapeutics through the formation of durable, target-specific interactions, and driving renewed interest across the pharmaceutical sector.

We developed a computational framework that integrates experimental structural data with AI-generated protein models to inform the design of covalent chemical tools and early-stage discovery starting points. This approach was applied to cereblon (CRBN), a clinically significant protein central to targeted protein degradation. Using this strategy, we designed novel chemical probes that enable the study of CRBN function and ligandability without the need for genetic modification of the protein.[1]

These findings demonstrate the potential of combining AI-derived structural insights with covalent ligand design to expand drug discovery and provide structural guidance for the development of probes to study disease-relevant biological mechanisms.

References

1. A. Khan, L. Diaz-Saez, L. Gerber, S. Warwood, D. Horton, P. J. Stansfeld, B. Wingelhofer, T. K. Britten and A. M. Lewis, *ChemRxiv*, 2026, DOI: 10.26434/chemrxiv.15002027.v1.

Development and implementation at 200kg scale of a transamination process

Jean-Marc Henry[1]

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Abstract: A novel active pharmaceutical ingredient (API) under development led to a series of synthetic challenges, which were addressed during process development to ensure successful production of clinical material.

Fig. 1 Scheme of transamination to intermediate 2

Prior to development, the synthesis of the target API required an exceedingly long cycle time. The main contributor was the transamination step, specifically the downstream removal of the large quantities of biological material required to promote the reaction. In addition to this, the dilute conditions required by the established enzyme and the low isolated yield led to an overall low throughput for this step. These shortcomings undermined the scalability and competitiveness of the process: the AstraZeneca team therefore worked to deliver a fast-paced process design work package to alleviate manufacturability concerns. Through rapid screening of alternative transaminase enzymes, a new biocatalyst was selected. After determining the optimal chemical space, the reaction was intensified with the aim to maximise substrate concentration. Near quantitative conversion of the ketone starting material at 50 g/L was achieved with an enzyme loading of 10 wt% by leveraging careful control of process parameters over the course of the reaction. Downstream removal of the biocatalyst through cellulose-assisted filtration was developed to ensure efficient purge of biological material before crystallisation and isolation of intermediate 2. This transamination process was successfully implemented at 20kg and 200kg scale in subsequent manufactures, thus enabling the synthesis of the required amount of API to support the clinical program, while greatly reducing the process mass intensity and the cycle-time compared to the initial process.

Plenary Lecture:

Mechanistic Understanding of Complex Catalytic Reactions Through a Temperature Scanning Protocol

Prof Donna Blackmond
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Professor Blackmond's research focuses on mechanistic studies of organic reactions, including asymmetric catalysis, and on the origin of biological homochirality.

Her team has carried out theoretical and experimental investigations that have helped to delineate models for how one enantiomer might have come to dominate over the other from what presumably was a racemic prebiotic world, highlighting both chemical and physical processes.
While much of the scientific driving force for this work arises from a fundamental interest in understanding the origin of life, research focusing on mechanisms for the enantioenrichment of chiral molecules has the potential to impact a wide range of applications, most notably in the synthesis and formulation of pharmaceuticals.

In 2025, she received the RSC Centenary Prize for Chemistry and Communication, awarded to outstanding chemists, who are also exceptional communicators, from overseas to give lectures in the UK and Ireland. Her prize was awarded *for her pioneering work in kinetic methods of organic catalysis, elegant descriptions of asymmetric catalysis mechanisms, insights into the origin of biological homochirality, and for excellence in communication.*

Poster Abstracts

Poster Contribution List

The numbering indicates the positioning of the posters.

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   PhotoDEL: Harnessing Light for on-DNA Chemistry

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   Applying a Catch-Edit-Release Strategy for the Late-Stage Homologation of C–N Bonds

3. **Carmen Barker-Benavides** Lancaster University
   Novel bis-pyridyl containing Pd Metal Organic Cages (MOCs)

4. **Samuel L. Brennan** University of Cumbria
   Squarilium Dyes in Photoantimicrobial Therapy: A Light-Driven Approach to Overcome Antimicrobial Resistance

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8. **Tom Edwards** Lancaster University
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9. **Ben Clarke** Lancaster University
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10. **Stefan Roesner** Liverpool John Moores University
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Poster Contribution List

The numbering indicates the positioning of the posters.

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12. **Andrei K. Zaitsev** University of Liverpool
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13. **Khaleel Zareen** Lancaster University
    Expanding Drug-Relevant Chemical Space Through Pt-Au Bimetallic Catalysis

14. **Guodong Ma** University of Liverpool
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15. **Philip J. Smith** Lancaster University
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16. **Debayan Roy** University of Manchester
    SmI_2-Catalyzed Coupling of Alkyl Housane Ketones and Alkenes in an Approach to Norbornanes

17. **Kevin Bucher** Lancaster University
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18. **Yuyi Man** Manchester Metropolitan University
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19. **Nilanjan Bhaduri** University of Manchester
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20. **Charlie Kenny** Lancaster University
    Surface Functionalisation with Arylimido-Polyoxometalates for Optoelectronic Applications

PhotoDEL: Harnessing Light for on-DNA Chemistry

Oliver J. Corrigan, Sarah L. Allinson, Jamie H. Docherty
Department of Chemistry, Lancaster University, Lancaster, LA1 4YB, United Kingdom
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Abstract: DNA-Encoded Libraries (DELs) have transformed early-stage hit discovery by facilitating the rapid screening of small molecules against biological targets.[1,2] In a DEL, each small molecule is conjugated to a unique DNA sequence that encodes its chemical identity, allowing for billions of compounds to be screened together against a chosen target. The challenge in constructing these large libraries lies in performing on-DNA chemical reactions in the presence of this DNA tag, with a limited range of reaction conditions being tolerated.[3] Due to these constraints, current libraries are typically limited to simple, sp^2-rich structures. Photochemistry and in particular Energy Transfer (EnT) catalysis offers a solution to this, allowing for the formation of complex, sp^3-rich structures under mild, DNA compatible conditions.[3] Here we present an efficient, on-DNA, EnT-catalysed [4+2] photocycloaddition reaction between a DNA-conjugated keto-naphthalene scaffold and a range of alkenes. This dearomative reaction affords a suite of bridged bicyclic products that can be incorporated into DELs and expand the chemical space coverage of these libraries and thus increase the chance of finding a successful hit upon screening.

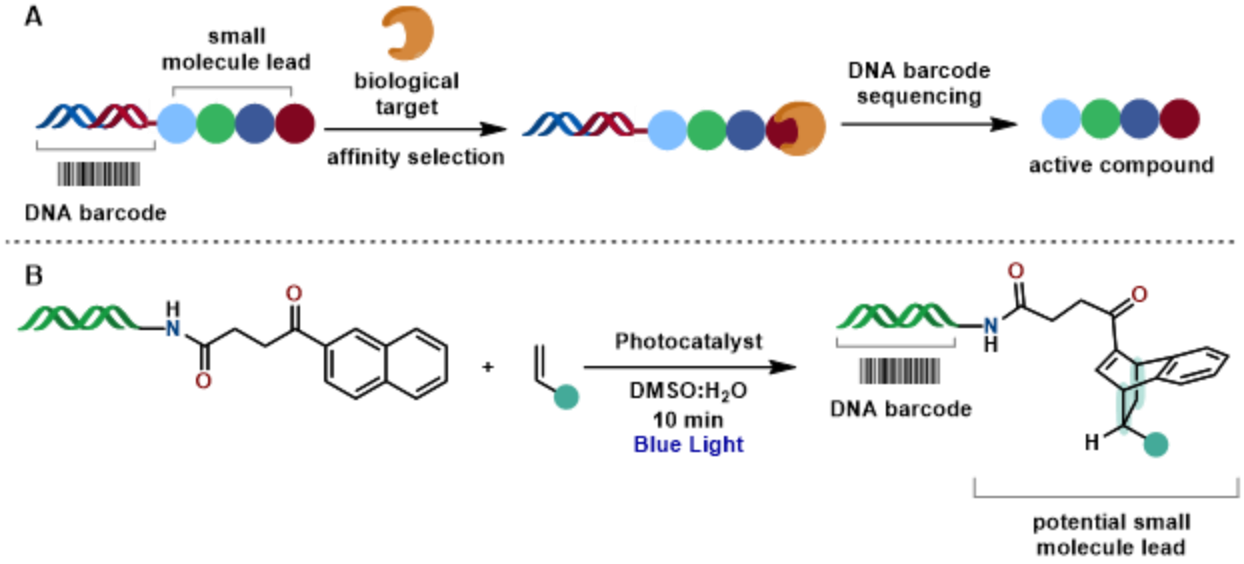

Fig. 1 - **A:** Discovery of an active pharmaceutical compound using DNA Encoded Libraries (DELs). The DEL consists of millions of small molecule lead compounds each with a unique DNA barcode. Affinity selection with a protein of interest allows for the selection of potential drug candidates which can then be identified by sequencing the unique DNA barcode. **B:** on-DNA [4+2] cycloaddition reaction between a DNA conjugated keto-naphthalene and a range of alkenes to generate a suite of small molecules that can be incorporated into DELS.

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Applying a Catch-Edit-Release Strategy for the Late-Stage Homologation of C–N Bonds

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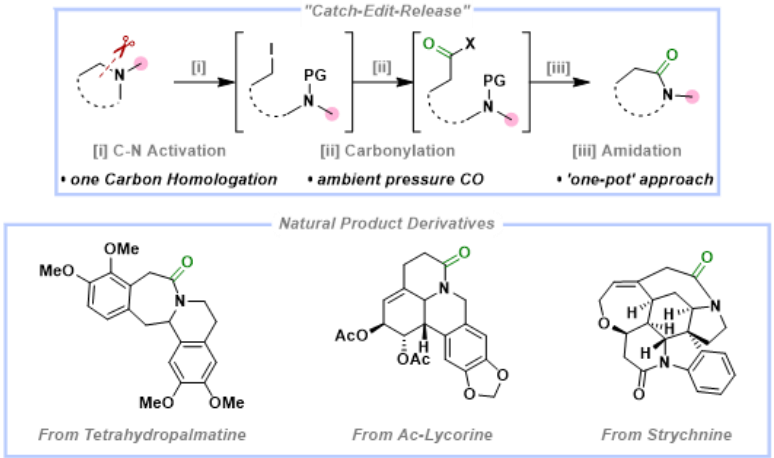
Abstract: N-Heterocycles are key components in many small molecule drugs and natural products. Around 75% of all biologically active compounds contain a *N*-heterocyclic moiety, and 65% of these are saturated.[1] This makes them ideal targets for late-stage diversity-oriented synthesis. The synthesis and modification of aromatic *N*-heterocycles has been explored extensively; however; their saturated counterparts offer unmet challenges. Recent methodological efforts have focussed on peripheral modifications, and skeletal editing processes that effect changes to the core structure remain rare.[2,3] Therefore, methods that selectively homologate such ring-systems on bioactive molecules to rapidly expand drug libraries are highly desirable.

Previous work on C–N activation within the Bower group,[4] has inspired a new "*Catch-Edit-Release*" strategy for the homologation of saturated *N*-heterocycles. This methodology utilises a three stage "one-pot" approach; *Catch*: C–N activation and ring-opening furnishes a versatile alkyl iodide intermediate.[4] *Edit*: A mild metal catalysed carbonylation of the C–I bond occurs under ambient CO pressure.[5,6] *Release*: *In situ* deprotection and recyclisation gives the homologated lactam product. This approach enables carbonylative homologations of 4-8 membered saturated *N*-heterocycles, including pharmaceutically relevant scaffolds and natural products.



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Novel bis-pyridyl containing Pd Metal Organic Cages (MOCs)

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Abstract: Metal–organic cages (MOCs) have emerged as promising supramolecular host structures for catalysts due to their ability to self-assemble, recognize substrates, and promote unique reactivity by confining molecules within well-defined nanoscale environments.[1] However, only a few have demonstrated catalytic activity and the scopes of in-cage reactions and enantioselective examples remains narrow. Bis-pyridines are one of the most common donor fragments for MOC design, with variations in the linker between the two donor atoms being key for cage size and shape. Chiral MOCs can be assembled by incorporating stereogenic centres into the polyhedral entities or inducing chirality through ligand twisting.[2] For example, studies on chiral self-sorting in Pd cages containing bis-pyridyl ligands derived from binaphthol and helicenes showed that spacer length affects self-sorting outcomes.[3] However, accessing new cage architectures using twisted ligand frameworks with potential for chiral self-sorting remains relatively underexplored.

This project aims to develop novel twisted ligand scaffolds for palladium MOC chiral self-assembly and explore their potential at the interface of catalysis and chemical biology. The project explores synthetic routes to access the twisted ligand, drawing inspiration from traditional transition-metal-catalysed cross-coupling chemistry and multistep organometallic synthesis previously developed in the group. By modifying the connectivity between the ligand backbone and coordinating donor groups, the work investigates how ligand geometry influences coordination to Pd(II) centres and the formation of discrete cage architectures. Subsequent self-assembly studies with palladium salts aim to identify conditions that favour cage formation, chiral self-sorting ability, and to probe the structural features that govern these processes.

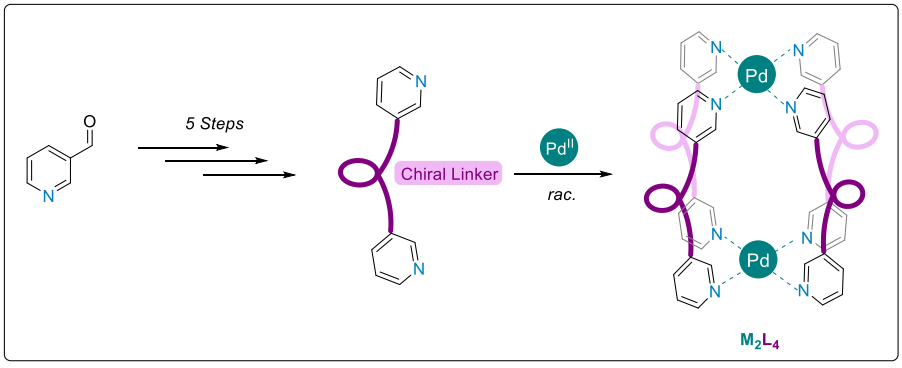

Fig. 1 Graphical Abstract.

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Squarilium Dyes in Photoantimicrobial Therapy: A Light-Driven Approach to Overcome Antimicrobial Resistance

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[1]University of Cumbria, Carlisle
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Abstract: Antimicrobial resistance is a global crisis, and typical systemic antimicrobial drugs brought to market quickly become obsolete due to their single mode of action, over prescription, and general misuse [1]. Photodynamic chemotherapy has highlighted how effective light sensitive organic dyes are at reducing tumour size and increasing rates of remission in cancer patients via the production of reactive oxygen species (ROS) [2,3]. Utilizing the same theoretical principles of ROS production, this study aims to explore the antimicrobial properties of *N*-substituted squarilium dyes, which exhibit strong molar absorption coefficients in the red-light region. Preliminary studies demonstrate therapeutically relevant minimum inhibitory concentrations (MICs) in the nanomolar range, underscoring the potential of these compounds as novel photoantimicrobial agents.

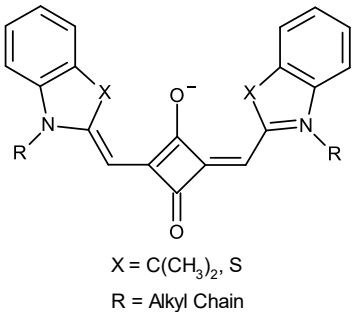

Fig. 1 Structure of Squarilium dye molecules

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Taking Inspiration from Nature: Displaying Biological Functionality in the Loop Region of [1]Rotaxanes as Synthetic Analogues of Lasso Peptides

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Abstract: In the search for new therapeutic agents, lasso peptides have emerged as promising candidates.[1] These naturally occurring peptides have [1]rotaxane-like motifs, where the mechanically interlocked macrocyclic 'ring' and axle are covalently attached to one another (Figure 1). Their self-tangled structures are believed to be imperative for their bioactivity; not only does the peptide chain show increased stability (in contrast to linear counterparts), but the interlocked nature also enforces specific conformational display of the amino acids within the 'loop' region. While the first chemical synthesis of a lasso peptide was reported in 2019,[2] this approach can be synthetically arduous. However, by using non-covalent template synthesis, both Coutrot,[3] and subsequently Bode,[4] have generated more accessible [1]rotaxane analogues. Here, we present our work on preparing families of [1]rotaxanes incorporating biological functionality (initially through amino acids) in the critical loop region. We have explored two approaches: (a) the cyclisation of a peptide attached to a [2]rotaxane scaffold[5] and (b) the expansion of the loop of a [1]rotaxane.[6]

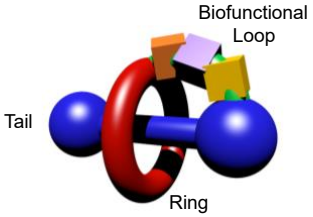

Fig. 1 Schematic of the components of a [1]rotaxane.

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PSDI Organic Toolkit: Introducing web services to report the reproducibility and scope of organic reactions

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Abstract: We introduce 'Organic Toolkit', developed by the UK Physical Sciences Data Infrastructure (PSDI) to assist researchers to adopt improved standards of reporting the reproducibility and scope of organic reactions.

Reaction yield is typically reported as a single value with no estimate of uncertainty that would enable others to judge the reproducibility of reported procedures. The PSDI Variability Plot Generator (https://organic-toolkit.psdi.ac.uk/variability-plot) is a secure browser-based tool to encourage reporting of reaction yield as its mean value accompanied by a confidence interval and variability plot. These provide interpretable measures of yield reproducibility and are also useful to identify outliers and prompt scrutiny of scale-up behaviour or sources of experimental variability. We demonstrate reporting of the uncertainty in yield for C-H carboxylation of substrates including benzothiazole, using Ph_3CCO_2K (Figure 1).[1]

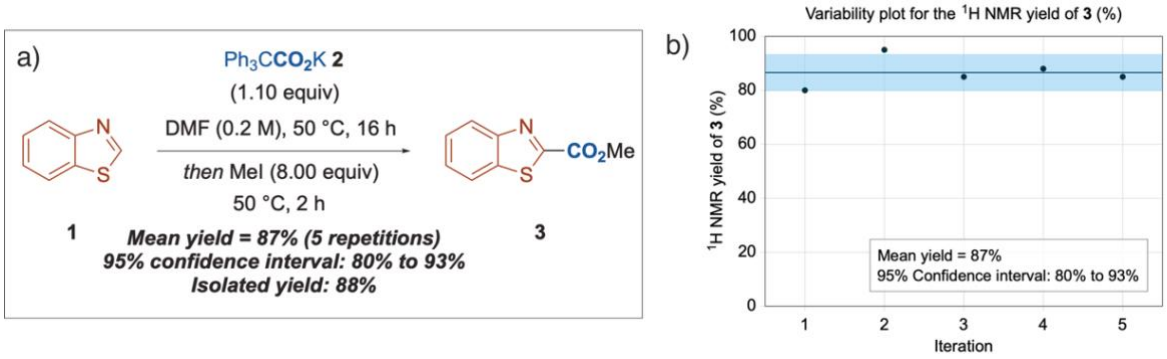
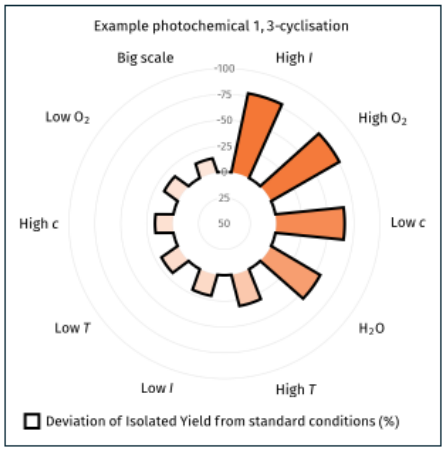


Figure 1 a) Carboxylation of benzothiazole. b) Variability plot for the NMR yield of **3** obtained using the PSDI Variability Plot Generator.



The Glorius Plot Generator (https://organic-toolkit.psdi.ac.uk/glorius-plot) depicts the sensitivity of any chemical transformation to user-defined reaction conditions, based on a concept from the Glorius group.[2] We introduce plot customisations and FAIR data export.

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Figure 2 Fan plot obtained using the PSDI Glorius Plot Generator.

Stereoselective Ir-catalysed α-Alkylation of γ-Lactams with Alkenes

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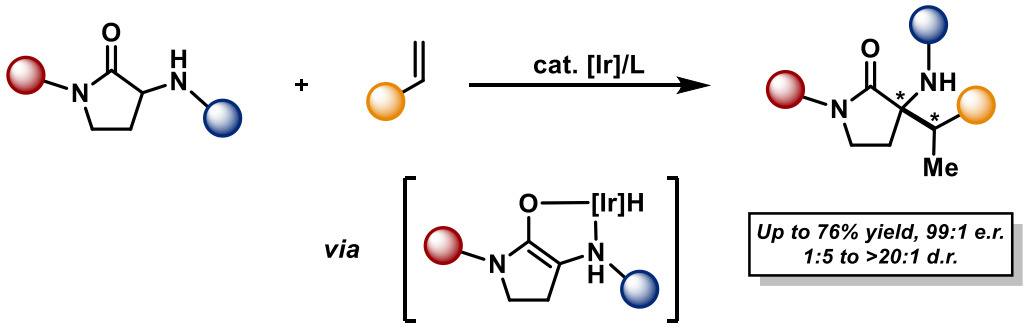
Abstract: The development of efficient methods to stereoselectively functionalise carbonyl compounds at the α-position is a long-standing objective in organic synthesis, owing to the ubiquity of these motifs in bioactive compounds and their utility as synthetic intermediates.[1] As an expansion to well-established chiral auxiliary methods, the development of new catalytic approaches has been crucial for the continued advancement of the field. Direct transition metal-catalysed methods of alkylation that do not require the pre-formation of enolates or enolate equivalents are uncommon, as are those that can utilise readily available alkenes as alkylating agents.[2,3,4] Furthermore, furnishing vicinal stereocentres in a stereocontrolled manner is highly challenging.[5]

This work, expanding on methodology previously developed in the Bower group, describes the by-product free α-alkylation of α-amino-γ-lactams *via* the stereoconvergent Ir-catalysed hydroalkylation of alkenes.[6] By harnessing an NH directing group strategy to facilitate the formation of an Ir-enolate intermediate, contiguous tetra- and tri-substituted stereocentres can be formed in a single step with high levels of diastereo- and enantioselectivity, and complete regioselectivity for the branched product. The reaction exhibits diastereodivergence based on the choice of lactam protecting group and the products generated can be further derivatised to generate sp^3 rich building blocks.



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A Solvent Solution to Selective Dewar Pyridone Formation

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Abstract: Bioisosterism is a fundamental concept in contemporary drug discovery where aromatic fragments in existing drug libraries are replaced with sp^3-rich heterocycles which maintain the same substituent orientation in space.[1] Bioisosteric replacement has been shown to enhance the pharmacophysical properties of this evolved series of drug candidates, presenting an opportunity to diversify drug discovery libraries. Current replacements use carbocyclic ring systems as scaffolds for *ortho* and *para*-isosteres, whilst similar *meta*-isosteres remain underrepresented.[1,2]

An unrealised class of *meta*-isosteric replacement are functionalised Dewar pyridones, incorporating heteroatom functionality which is absent in the current isosteric chemical space. The parent Dewar pyridone scaffold can be generated from medicinally privileged 2-pyridones *via* a [4π] – photocyclisation.[3] However, a long standing issue is the competing [4π + 4π] dimerisation of 2-pyridones under photochemical conditions, reducing the achievable yield of this highly desirable Dewar heterocycle.[4] Utilising the unique reactivity profile of 1,1,1,3,3,3-hexafluoroisopropanol (HFIP), we have suppressed unproductive [4π + 4π] dimerisation to selectively afford Dewar pyridones, overcoming the previously apparent upper yield limit.[3,5] This synthetic innovation serves as a platform for the unhindered generation of Dewar pyridone scaffolds which could be diversified to generate libraries of viable *meta*-isosteric replacements.

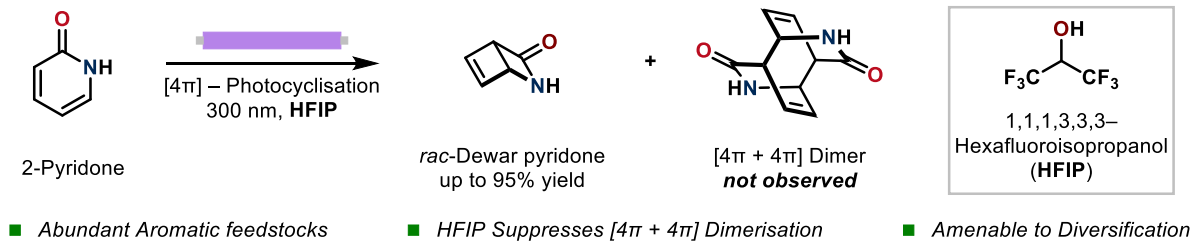

Fig. 1 [4π] – Photocyclisation of 2-pyridones to selectively afford Dewar pyridones over competing dimerisation.

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The Design & Synthesis of Fluorescent Self-Assembled Monolayers for Optical Applications.

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Abstract: Controlling the orientation of π-conjugated molecules is an important area of research, as molecular orientation plays a critical role in determining the efficiency of optoelectronic devices.[1] Many high-performance devices are currently fabricated using vacuum evaporation techniques, which are energy intensive and suffer from extremely low material utilisation.[2]

In this work, we introduce a novel approach towards controlling molecular orientation based on greener, solution-processed methods. The control of tilt angle within self-assembled monolayers (SAMs) is exploited to influence the orientation of π-conjugated molecules at metal oxide interfaces. A series of carbazole donor–acceptor emitters were designed and synthesized, before monolayers were deposited onto indium tin oxide (ITO) substrates. Their structures were investigated using a combination of surface characterisation techniques. These techniques reveal high binding efficiencies, and the effects of deposition parameters and post-deposition treatment on film quality and surface coverage were also examined. Photophysical studies show bright blue charge-transfer emission with solvatochromic behaviour, while solid-state measurements are ongoing but indicate bright emission.

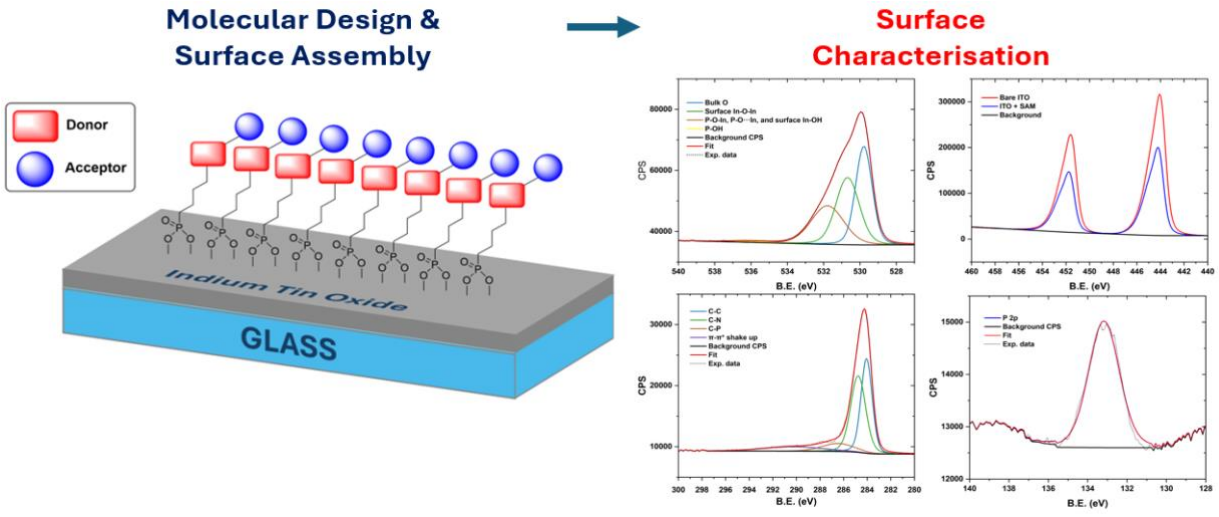

Fig. 1 Left: Schematic representation of donor–acceptor self-assembled monolayers (SAMs) on ITO. Right: XPS spectra confirming SAM binding to the ITO surface.

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Synthesis of sp^3-rich Cyclic Hydrazine Frameworks for Drug Discovery

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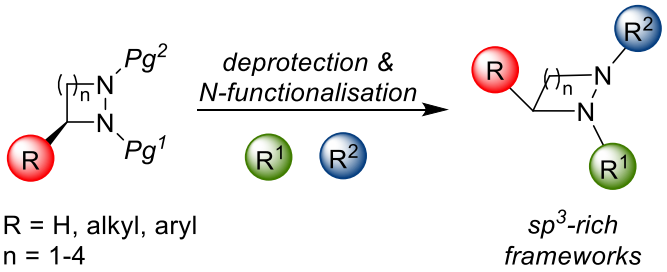
Abstract: It has been demonstrated that increased molecular complexity correlates with improved chances of success in the drug discovery process, as it enhances bioavailability and target specificity.[1,2] Here, strategies for the synthesis of sp^3-rich, non-planar heterocyclic scaffolds suitable for drug discovery are described. Employing diverse synthetic strategies, we synthesise orthogonally protected, enantiomerically enriched cyclic hydrazines bearing varied C-3 substituents. Through iterative C–N functionalisation, we generate structurally diverse libraries, leveraging a broad range of chemistries and coupling partners. NMR and crystallographic studies confirm that these frameworks display significant sp^3-character, with the nitrogen substituents adopting an anti-configuration under the control of a single stereogenic centre, exploiting the fluxional behaviour of the two nitrogen atoms. This strategy is applied to the synthesis of 1,2-diazetidines[3] and larger cyclic hydrazine frameworks.[4]



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Directing Oligomeric Intermediates in Cucurbituril Synthesis

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Abstract: The condensation of glycoluril with formaldehyde to form cucurbiturils is a highly condition-dependent process, where subtle variations can shift the outcome between discrete macrocycles and lower oligomeric species. In this work, we investigated how altering the reagent ratio under acidic conditions affects the reaction pathway and product distribution. Instead of promoting direct macrocycle formation, the reaction parameters were tuned to favor the generation of early-stage oligomers. These intermediates were successfully isolated and characterized by NMR and IR spectroscopy, with structural assignments based on diagnostic signals from terminal functionalities and distinctive methylene resonances. Our findings reveal that the availability of formaldehyde is a key factor governing the assembly process, providing a practical means to control product selectivity. Overall, this study underscores the importance of intermediate species in cucurbituril synthesis, offering insights that can enhance synthetic strategies and deepen understanding of macrocycle formation mechanisms.

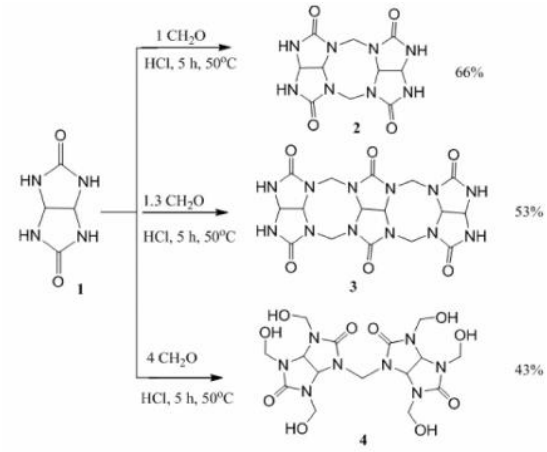

Fig. 1 Synthesis of oligomers

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Base-catalysed linear-selective addition of amino acids to vinyl arenes

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Abstract: Unnatural amino acids (UAAs) attract great interest due to their potential applications in drug design[1], biocatalysis[2] and synthetic biology.[3] An important UAA scaffold, composed of glycine and phenethyl units is found in several commonly-prescribed drugs.[4] An Ir-catalysed branch-selective hydroalkylation with styrenes, previously developed in our group, affords similar structures,[5,6] however, a direct synthesis of linear glycine-styrene fragment from achiral materials is unknown. Here a new linear-selective method based on base-catalysed addition of various electronically diverse vinyl arenes to *N*-protected glycinamides is presented, providing access to a wide range of UAAs. The reaction is in line with previously reported *C*-alkylations of K enolates with styrenes, commonly abbreviated as CAKES.[7] It was demonstrated that the reaction can be performed efficiently and selectively in mild conditions, i.e. room temperature and catalytic amounts of KHMDS, generally 5 mol. %. A combination of potassium *tert*-butoxide and crown ether afforded the reaction between mono-addition products and second equivalent of styrene, providing α,α-disubstituted amino acids. Several chiral crown ethers were synthesised and tested as ligands in attempt to perform the reaction asymmetrically, however, none of them were successful.

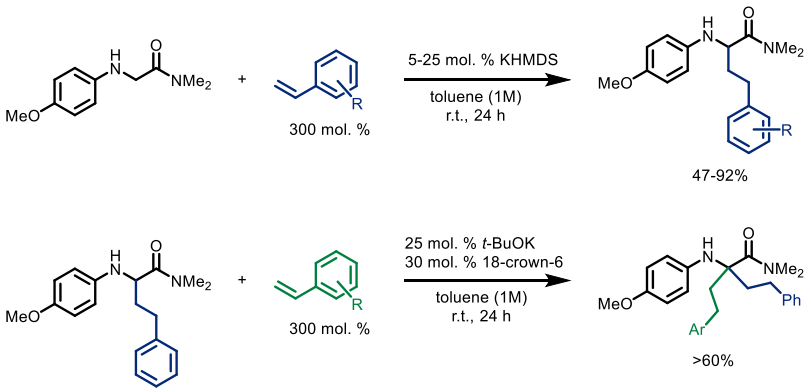

Fig. 1. Mono- and double addition of amino acid dimethyl amides potassium enolates to vinyl arenes.

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Expanding Drug-Relevant Chemical Space Through Pt-Au Bimetallic Catalysis

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Abstract: Bimetallic catalysis has evolved in recent years as a powerful strategy towards the synthesis of new structures, inaccessible through monometallic systems. Homogeneous Pt-Au bimetallic catalysis has scarcely been reported on, limited to only a few reported examples by Muñoz and co-workers, each proceeding via different mechanisms: cooperative regioselective 1,3-double addition of azoles to terminal allenes,[1] and a tandem Au-catalysed *N*-indolylallene cyclisation followed by Pt-Au bimetallic clusters regioselectively controlling the nucleophilic addition of indoles and azoles.[2,3] 1,6-Enynes have been known to undergo several different reactions, including the nucleophilic addition of indoles.[4] Under Pt-Au bimetallic catalysis, a rapid, tandem, orthogonal, one-pot synthesis of cyclopropyl-containing bis(indolyl)methanes (BIMs) has been uncovered from TsN-tethered 1,6-enynes.[5] These novel, indole- and azole-containing compounds are promising structures in the quest to explore new chemical space for drug discovery, and some have already shown powerful antimicrobial and selective anticancer properties.[6]

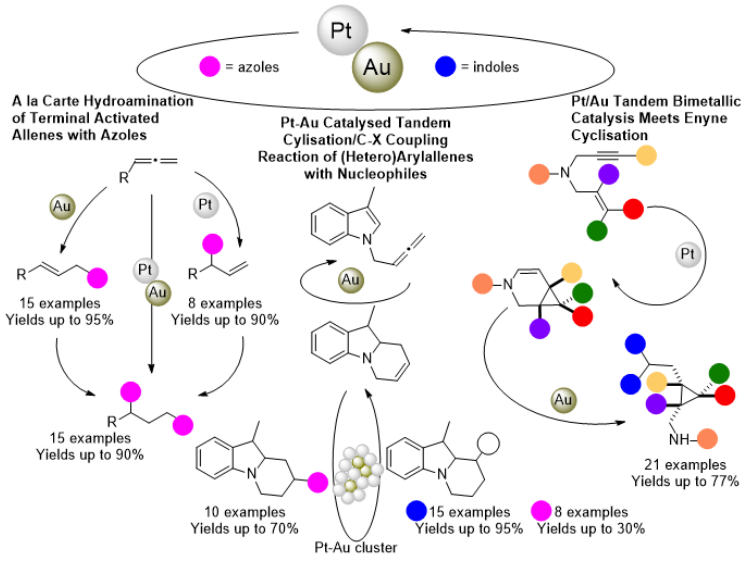

Fig. 1 Overview of Pt-Au bimetallic catalysed systems.

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Leveraging alkenyl boron reagents for stereoselective, diversity-oriented synthesis

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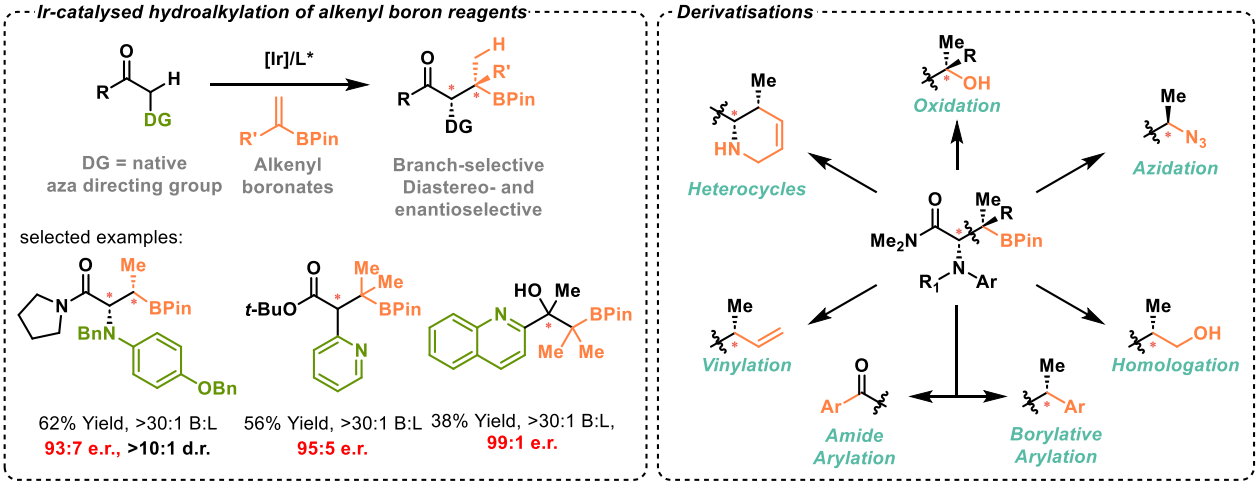
Abstract: The global amino acid market is experiencing rapid growth due to the increasing demand in pharmaceutical and drug development, organic catalysts and specialty chemicals, medical nutrition and cosmetics.[1] Current synthetic methods enable facile access to relatively simple natural and unnatural amino acids. However, production of more complex amino acids requires inefficient alternative routes, often starting from the chiral pool and requiring chiral resolution in their synthesis. Most significantly, the synthesis of α-amino acids bearing additional β-substitution remains a significant challenge and methods that can install the α-C(sp^3) –C(sp^3) bond in a stereo-controlled manner remain extremely scarce.

Here, we report an iridium(I)-catalysed C(sp^3)–H addition of a range of pronucleophiles to alkenyl boronates, based on a directed enolization strategy previously developed in the Bower group.[2,3] This approach allows access to α-amino acid derivatives with a chiral boron centre at the β-position, with extremely high levels of diastero- and enantioselectivity, complete branch selectivity and high atom economy.[4] The boron handle can be derivatised to a wide range of useful different structures, allowing access to to a variety of high-value, unnatural amino acids that are challenging to access stereoselectivity with other methods.



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A Pyridone Photoswitch Stores Heat at 1.3 MJ kg^{-1} with 365 nm Light Charging

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Abstract: Molecular solar thermal (MOST) systems store solar energy as chemical potential in a photoisomer and release it later as heat in a closed cycle, offering deployable thermal energy without thermal insulation. Here we report a simple natural product pyridone photoswitch that undergoes a [4π]-photocyclisation to a Dewar isomer under 365 nm irradiation and can be repeatedly charged and discharged over multiple cycles. Differential scanning calorimetry measures an energy storage density of 1.32 MJ kg^{-1}, placing this compact scaffold among the highest-energy MOST candidates while operating in the UVA band relevant to terrestrial sunlight. Ground state calculations locate the thermal reversion transition state ($\Delta G^{\ddagger}$ = 32.4 kcal mol^{-1}), suggesting a half-life of 2000 years at 298 K. These results establish pyridone Dewarisation as a high-strain MOST platform that couples MJ kg^{-1}-class energy density with UVA charging and long-term kinetic stability, opening a route to compact molecular materials for sunlight-driven heat storage.

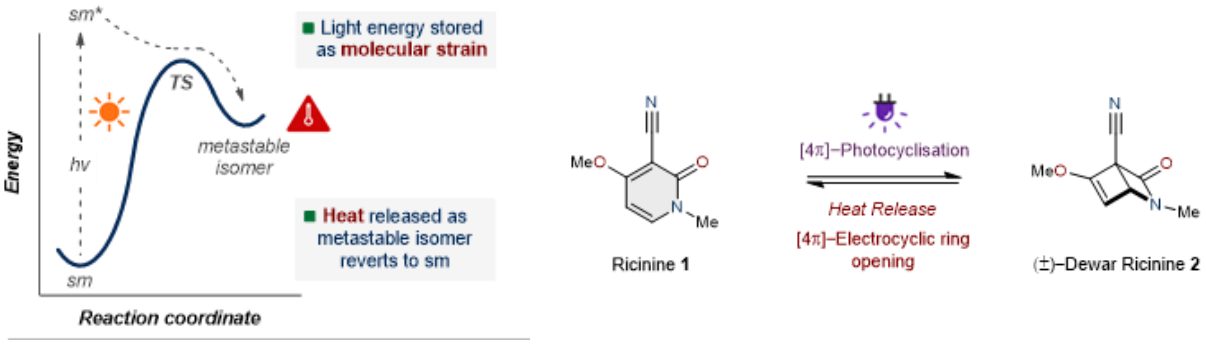

Fig. 1 Left: Schematic energy profile showing light-driven formation of a metastable isomer that stores energy as molecular strain and releases heat on thermal back-conversion to the starting material (sm) & Right: Ricinine **1** undergoes thermally-reversible Dewarisation.

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SmI_2-Catalyzed Coupling of Alkyl Housane Ketones and Alkenes in an Approach to Norbornanes

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Abstract: Strain-release strategies in cross-coupling chemistry have emerged as powerful tools for constructing complex, three-dimensional molecular architectures, particularly in the design of bioisosteres for medicinal chemistry. While significant effort has been invested in developing strain-release chemistry of cyclopropanes[1-4] and bicyclo[1.1.0]butanes,[1,2,5-8] the reactivity of higher homologues remains underexplored. In this work, we report a mild and atom-economical samarium diiodide (SmI_2)-catalyzed fragmentation and coupling of bicyclo[2.1.0]pentane (housane) ketones with electron-deficient alkenes.[9] This method proceeds under mild conditions and enables recalcitrant alkyl housane ketones to be engaged in addition to more reactive aryl substrates, thus expanding the current substrate scope for housane-based transformations.[10] The reaction allows efficient access to functionalized norbornane frameworks that are challenging to obtain through conventional two-step Diels-Alder cycloaddition-reduction strategy due to electronic mismatching. Products offer versatile handles for downstream functionalization, highlighting the potential of this approach for the synthesis of structurally complex sp^3-rich, conformationally defined, 3D architectures and medicinally relevant scaffolds.

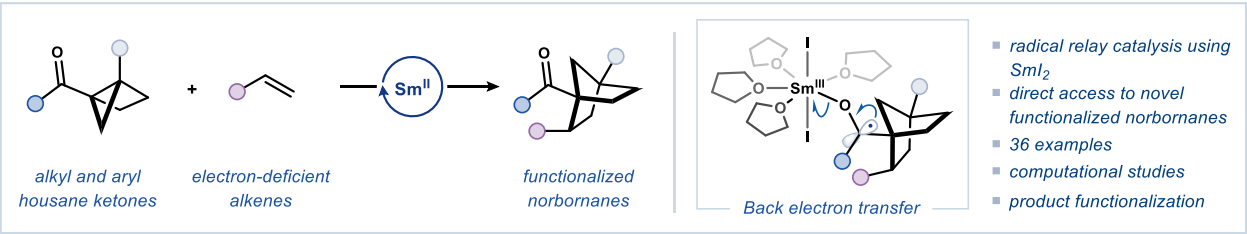

Fig. 1 SmI_2 catalyzed coupling between housane ketone and alkenes through radical relay approach.

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Iron-porphyrin Catalyzed Deaminative Hydrobenzylation of Alkenes using Redox-active Pyridinium Salts

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Abstract: All-carbon quaternary centres are valuable motifs in medicinal chemistry because their increased sp^3 character enhances molecular complexity, conformational rigidity, and properties such as solubility, metabolic stability, and selective protein binding, yet they remain challenging to access using conventional two-electron synthetic methods.[1-3] Radical cross-coupling strategies, particularly those combining metal-hydride hydrogen atom transfer (MHAT) with iron-catalysed radical coupling, have provided efficient routes to $C(sp^3)$–$C(sp^3)$ bond formation from alkenes.[4-8] Here, we report a deaminative hydrobenzylation method that merges MHAT with a reductive pathway using readily accessible N-benzylpyridinium salts and a commercially available iron–porphyrin catalyst. The protocol enables efficient construction of all-carbon quaternary centres across 62 examples (25–92% yield), while mechanistic studies support a radical pathway involving electron donor–acceptor (EDA) complex formation. The operational simplicity, broad substrate scope, and mechanistic insight highlight the potential of this platform for late-stage functionalisation and rapid synthesis of drug-relevant scaffolds.

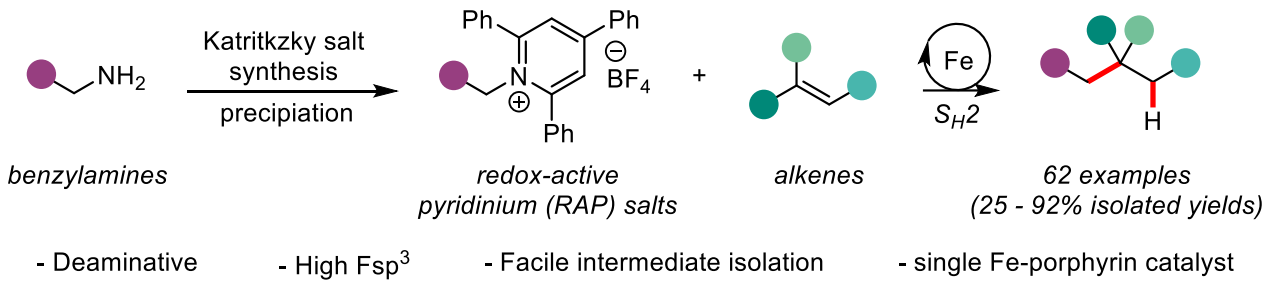

Fig. 1 Deaminative hydrobenzylation of alkenes via MHAT/SH2 catalysis enables efficient synthesis of all-carbon quaternary centres from benzylic amines.

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Photoinduced C(sp²)-C(sp³) Cross-Coupling for the Diversification of Non-Thalidomide Cereblon E3 Ubiquitin Ligase Binders

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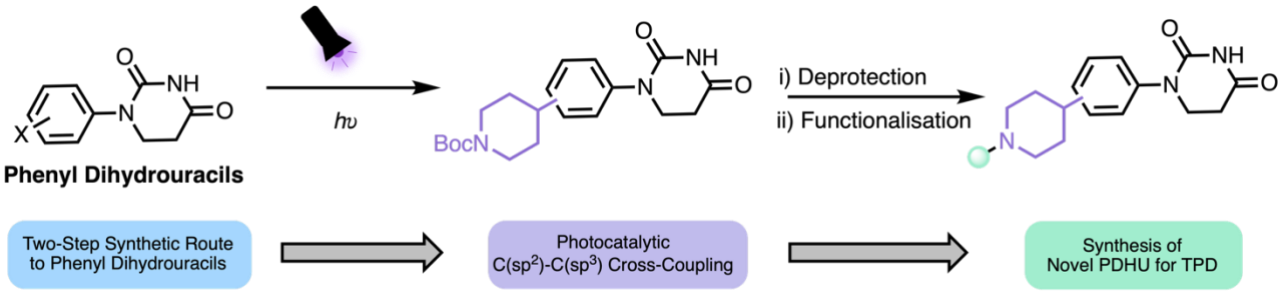
Abstract: Cancer remains one of the leading causes of mortality worldwide, accounting for approximately 10 million deaths annually. A key limitation of many current therapeutics is their inability to selectively target cancerous over healthy cells. Modulation of the ubiquitin–proteasome system (UPS) has therefore emerged as an alternative strategy for the selective degradation of oncogenic proteins. Early exploitation of the UPS was achieved through immunomodulatory drugs (IMiDs) such as thalidomide and its derivatives, which act by hijacking the E3 ubiquitin ligase cereblon (CRBN) to recruit and degrade protein substrates (neosubstrates) that would not otherwise interact with CRBN. However, IMiDs suffer from pharmacokinetic liabilities and teratogenic effects, motivating the development of structurally distinct non-thalidomide CRBN binders (such as phenyl glutarimides, phenyl dihydrouracils).[1]

Herein, we report a photoinduced C(sp²)–C(sp³) cross-coupling methodology, previously applied to thalidomide-derived CRBN binders,[2] for the diversification of non-thalidomide cereblon E3 ubiquitin ligase binders. Upon irradiation, a Hantzsch ester acts as a stoichiometric reductant to generate carbon-centred radicals, which undergo nickel-catalysed cross-coupling to introduce sp³-rich fragments onto phenyl dihydrouracils, affording structurally diverse analogues that contain functional groups to enable downstream applications towards bifunctional proteolysis targeting chimeras (PROTACs).



Scheme 1 *X = Halogen (Br or I) , = Linker for Bifunctional Degraders; PDHU = Phenyl Dihydrouracils; TPD = Targeted Protein Degradation*

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Trifluoromethylation of Pyridines through Skeletal Rearrangement

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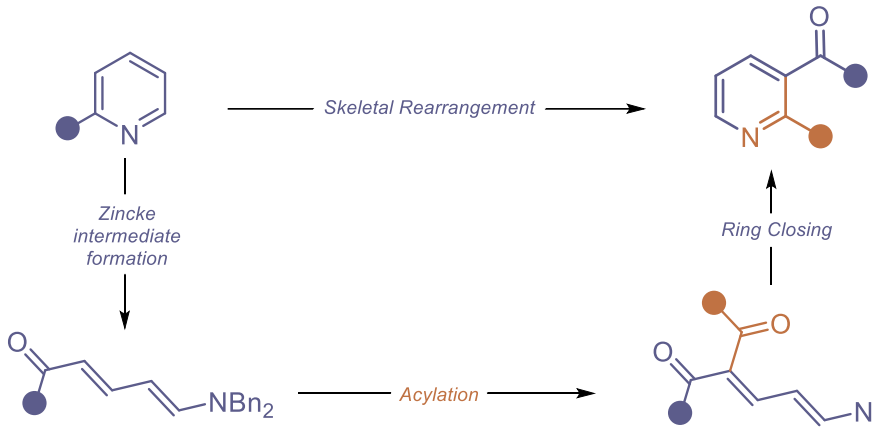
Abstract: A novel pyridine skeletal rearrangement has been developed that enables selective functionalization at the challenging C2 position through Zincke intermediates, along with the installation of valuable 3-(*het*)aroyl and 3-formyl substituents. Pyridines are first converted into ring-opened Zincke intermediates,[1,2] which undergo regioselective fluoroacylation with inexpensive, readily available fluorinated acylating agents. Subsequent ammonia-mediated ring closure proceeds through an alternative cyclization pathway to furnish rearranged pyridines bearing the valuable electron-poor substituents, including CF_3, CF_2H, and CO_2Et at the C2 position. The method provides a practical and highly selective route to C2-trifluoromethylated pyridines, overcoming the poor C2/C4 selectivity commonly encountered in conventional Minisci-type radical functionalization. A broad substrate scope was demonstrated, including aryl-, heteroaryl-, and fused heterocyclic pyridines, as well as medicinally relevant scaffolds.



- Zincke chemistry - C2 fluoroalkylation - C3 aroylation/formylation - Rearranged trifunctional pyridines -

Importantly, the rearrangement simultaneously converts the original C2 substituent into synthetically versatile 3-aroyl functionality, while C4-substituted pyridines generate corresponding 3-formyl derivatives - a valuable synthetic handle for further derivatisation. The nucleophilic nature of the Zincke intermediates further enabled sequential electrophilic functionalization, allowing efficient synthesis of densely substituted 2,3,4- and 2,3,5-trisubstituted pyridines through Heck arylation[3] and halogenation strategies[2]. This work established ring-opening/ring-closing skeletal editing as a versatile platform for selective pyridine diversification and the synthesis of fluorinated heterocycles.[4]

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Surface Functionalisation with Arylimido-Polyoxometalates for Optoelectronic Applications

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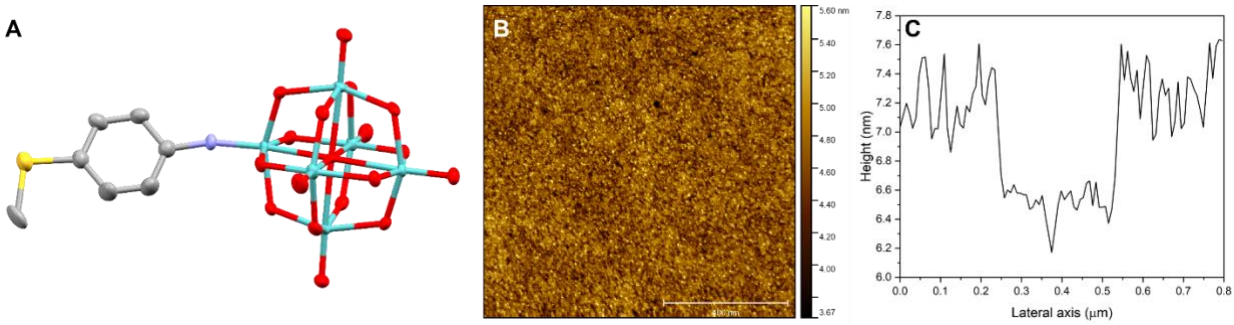
Abstract: Functionalization of polyoxometalates (POMs) with arylimido groups results in the formation of hybrid materials with strong electronic communication between the organic and polyoxometalate moieties. This communication can produce charge transfer systems that display non-linear optical properties,[1-3] with high visible transparency and the capacity for redox switching[3] – all demonstrated in solution. Our goal now is to translate this work to surfaces suitable for optoelectronic devices, and investigate the electronic (charge transport) and optical properties of the resulting films in different redox states. In this poster, we will present synthesis of several arylimido-POMs bearing surface binding groups such as-SMe (Figure 1A), and preliminary investigation of functionalization of Au (Figure 1B, C) and other surfaces.



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