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Short Abstracts of Interesting Recent Publications of Swiss Origin

High-Throughput Iridium-Catalyzed C–H Borylations for Rapid Investigation of Heterocyclic Fragments in Discovery Chemistry

Clara Muller, Simone Kuhn, Sharon Bell, Richard Kraus, Thomas Stadelmann, Tomas Smejkal, Julien C. Vantourout, and Daria Grosheva

Helvetica Chim. Acta **2025**, e00096.
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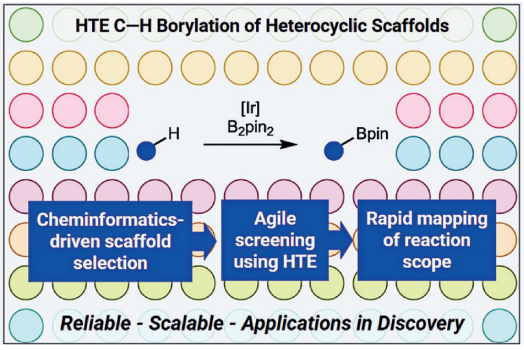
Research Chemistry, Syngenta Crop Protection AG, Schaffhauserstrasse 101, Stein, AG, 4332 Switzerland

Ir-catalysed C–H borylation has become a powerful tool in drug discovery and agrochemistry, particularly for late-stage functionalisation of heterocycles. However, most studies report only narrow substrate classes, making it difficult to broadly evaluate the method's applicability across structurally diverse scaffolds relevant to lead optimisation. In this study, a systematic workflow was established to assess Ir-catalysed C–H borylation across bicyclic *N*-heteroarenes. Representative scaffolds from this chemical space were clustered and selected with cheminformatics, then screened under varied catalytic conditions on a high-throughput experimentation (HTE) platform. This strategy uncovered substrate-specific catalytic systems and regioselectivity patterns that could not easily be predicted in advance. By combining cheminformatic-driven design, HTE screening, and rapid scale-up validation, this approach enables efficient mapping of reaction scope. The results demonstrate a practical method to identify robust conditions for challenging heterocycles, providing a strong framework to accelerate synthetic methodology development and streamline lead optimisation in pharmaceutical and agrochemical research.

Authors' comments:
"Using cheminformatics, we first selected a diverse set of molecular scaffolds to evaluate their performance in a specific reaction class. Our automation platform then enabled rapid identification and subsequent scale-up of optimal conditions. This strategy can be systematically applied across multiple research projects."



Structure and Catalytic Properties of Homo- and Heterometallic Iron(II)-Based di(2-pyridyl)ketone Oxoclusters

Daniel R. Civettini[a], Carlos A. Triana[a], Tjeerd F. De Jong[a], Daniel F. Abbott[b], Robin N. Dürr[b], Sandra Luber[a], Victor Mougel[a], and Greta R. Patzke[b]

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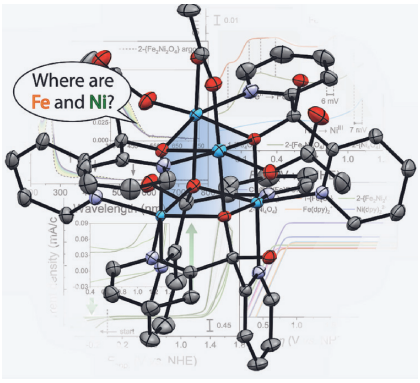
https://doi.org/10.1021/jacs.5c04262
[a]University of Zürich; [b]ETH Zürich

Patzke *et al.* report on the synthesis and characterisation of two new iron(II)-based oxoclusters, a homometallic 1-{Fe_4O_4} and a heterometallic 2-{$Fe_2Ni_2O_4$}, as catalysts for oxygen evolution reaction (OER). 2-{$Fe_2Ni_2O_4$} cubane is the first molecular model of the crucial {H_2O–$Fe_2Ni_2(OR)_2$–OH_2} motif found in highly active Ni/Fe oxide-based heterogeneous catalysts. Advanced techniques, including X-ray absorption spectroscopy, neutron scattering, and computational models, confirmed the precise alternating arrangement of Fe(II) and Ni(II) ions within the metallic core. This heterometallic oxocluster reveals synergistic effects, tuning the redox potentials of both metals and enhancing the stability of the oxidized precatalyst species. Electrocatalytic testing showed that 2-{$Fe_2Ni_2O_4$} outperforms its homometallic counterparts, achieving a maximum catalytic current density of 1.75 mA/cm^2 and a high Faradaic efficiency of 84.8% for OER with no significant formation of inactive metal (oxy)hydroxide particles. 2-{$Fe_2Ni_2O_4$} is a valuable platform for future in-depth mechanistic studies of the synergistic interactions between Ni and Fe, which are critical for designing efficient, earth-abundant OER catalysts.

Authors' comments:
"The study reports on new homo- and heterometallic cubanes, 1-{Fe_4O_4} and 2-{$Fe_2Ni_2O_4$}, mimicking enzymatic sites and oxides OER catalysts. Structural and electrochemical analyses highlight Ni/Fe synergies that fine-tune redox properties and enhance OER activity."



Prepared by Cesare Berton, James Southwell, Titouan Chetot, Jonas Genz, Stanislav Prytuliak, Fan Liu, Eda Nisli, Deborah Bäcker, Samy Kichou, Dominik Roth, Laura Schüpke, Jan Vetterli, Henrik Braband, and Jason P. Holland*
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Size-Selective Functionalization of Sugars and Polyols Using Zeolites for Renewable Surfactant Production

Songlan Sun, Zezhong J. Li, Yu-Cheng Lin, Manon Rolland, Tom Nelis, Seongmin Jin, Shasha Zheng, Benjamin N. Raffy, Wen H. Bi, Esther Amstad, and Jeremy S. Luterbacher*

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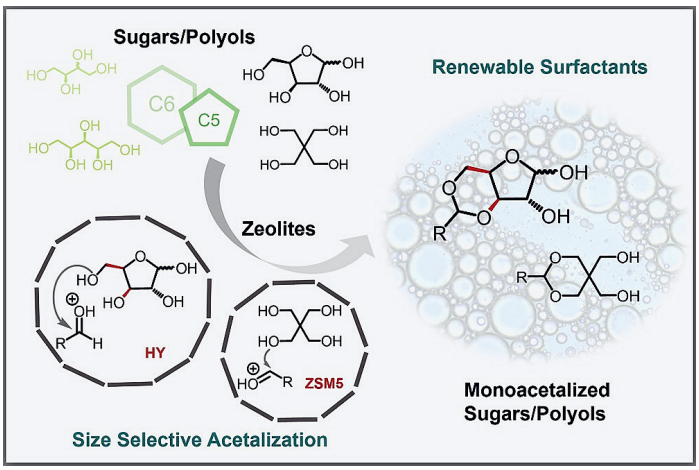
https://doi.org/10.1002/anie.202511282

Laboratory of Sustainable and Catalytic Processing, Institute of Chemicals Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne CH-1015, Switzerland

This study presents a novel catalytic method for the selective modification of sugar and polyol molecules *via* acetalization. Conventional techniques for this type of reaction often require inefficient, multi-step processes to achieve selectivity. The research demonstrates that using zeolites as catalysts enables precise, single-step functionalization governed by controlled pore confinement. By strategically matching the dimensions of the reactant and the product to the zeolite's internal structure, the process reliably produces mono-functionalized compounds in high yields. These novel monoacetals serve as effective building blocks for bio-derived surfactants. Performance testing revealed that these surfactants, particularly those derived from xylose, match or exceed the functionality of conventional petroleum-based options, demonstrating exceptional stability in hard water while being biodegradable. This approach provides a streamlined and sustainable pathway for creating valuable chemicals from renewable resources.

Authors' comments:
"The ability to precisely control sugar acetalization selectivity marks another important step in our effort to functionalize biomolecules with minimal structural alterations, paving the way for high-performance, easy-to-produce chemicals and materials."



A Supramolecular Nanosheet Assembled from Carpyridines and Water

Joseph F. Woods, Kai Zhang, Joëlle Peterschmitt, Olivier Blacque, Céline Besnard, Gustavo Santiso-Quinones, Laura Samperisi, Andreas Vargas Jentzsch, and Michel Rickhaus*

J. Am. Chem. Soc. **2025**, *147*, 18380.
https://doi.org/10.1021/jacs.4c17024

Department of Chemistry, University of Zurich, CH-8057, Zurich, Switzerland; Department of Organic Chemistry, University of Geneva, CH-1205, Geneva, Switzerland

This study reports the first crystallographic evidence of water acting as a monomer in supramolecular materials. Phenylated carpyridines assemble into nanosheets whose structures depend strongly on water content. In dry toluene, π–π interactions stabilize antiparallel stacks, while in wet conditions, water molecules insert into the macrocyclic cavity, creating hydrogen-bonded linear columns with porous 1D channels. Cryo-electron diffraction at 100 K of samples from regular toluene revealed a structure intermediate between wet and dry phases, indicating semistable states. Annealing in dry toluene converted the wet phase to the dry polymorph, while the reverse required dissolution into the monomers and reassembly in wet toluene. The relatively new technique of electron diffraction crystallography was crucial to resolve the structures. The porous nanosheets present opportunities in host–guest chemistry, gas adsorption, and water-responsive supramolecular design.

Authors' comments:
"This work shows how subtle solvent changes can locally reorganize entire self-assemblies, while macroscopically, they remain indistinguishable by microscopy. This underscores the crucial role micro-ED can play to advance our understanding of supramolecular polymer chemistry at the molecular organisation level."