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Swiss Science Concentrates

A CHIMIA Column

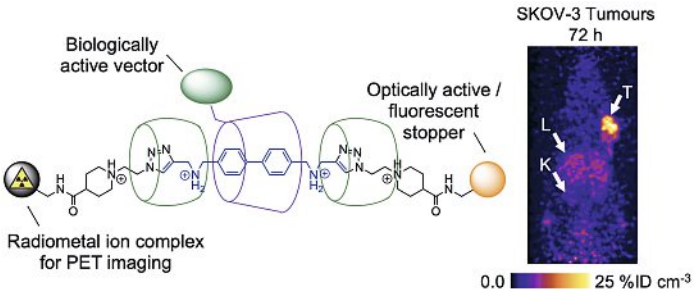
Short Abstracts of Interesting Recent Publications of Swiss Origin

Supramolecular Rotaxane-Based Multi-Modal Probes for Cancer Biomarker Imaging

Faustine d'Orchymont and Jason P. Holland*,
Angew. Chem. Int. Ed. **2022**, e202204072
https://doi.org/10.1002/anie.202204072
University of Zurich

Interlocked molecules present opportunities to construct therapeutic drugs and diagnostic imaging agents but making these biologically active probes in water is challenging. Herein the authors report the development using self-assembly methods and a rotaxane-based approach to create radiolabelled and optically active species that can be conjugated to cancer-targeted monoclonal antibodies or peptide-based drug molecules. Tumour-specific uptake of supramolecular rotaxane-based radio-labelled mAb was observed *in vivo* where PET imaging and biodistribution analysis was used to study pharmacokinetics of [^{89}Zr]ZrFe-[4]rotaxane-trastuzumab. They also demonstrated the ease of tuning the system by varying the rotaxane architecture, which provides compelling evidence that rotaxane-based supramolecular chemistry is a versatile platform for designing molecular imaging probes that target biomarkers of disease.

Authors' comments:
"In radiopharmaceutical design, methods to reduce organ dosimetry are crucial. Self-assembly using non-covalent mechanical bonds offers new ways of controlling the distribution, metabolism, and excretion profile of radiotracers *in vivo*."

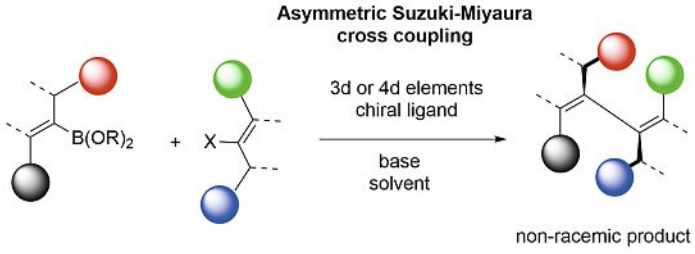


The Catalytic Formation of Atropisomers and Stereocenters *via* Asymmetric Suzuki-Miyaura Couplings

Gaspard Hedouin, Suzanta Hazara, Fabrice Gallou, and Sachin Handa*, *ACS Catal.* **2022**, *12*, 4918–4937
https://doi.org/10.1021/acscatal.2c00933
Chemical & Analytical Development, Novartis Pharma AG, CH-4056 Basel

The Suzuki-Miyaura reaction is one of the most versatile and commonly used cross-coupling reactions. However, asymmetric applications to deliver highly functionalized atropisomers or nonracemic coupling products, are much less widely reported. Although there has been some notable work utilizing asymmetric Suzuki-Miyaura reactions, there continue to be significant obstacles to its effective use, in particular, when preparing highly functionalized heterocyclic atropisomers. Medicinal chemistry applications in this area will undoubtedly fuel the discovery of novel and practical solutions to combat this problem. This review focuses on the use of asymmetric Suzuki-Miyaura cross coupling reactions to aid heterocyclic and homogeneous catalysis reactions.

Authors' comments:
"The selective generation of atropisomers has become a superb playground for the development of impactful sustainable catalytic cross-coupling methodologies, whether using base metals, or sustainable media.



Prepared by David Lim, David Roura Padrosa, Gordon Honeyman, Keir Penston, and Francesca Paradisi*
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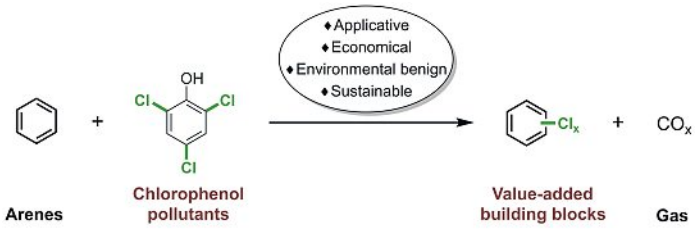
Chlorination of Arenes *via* the Degradation of Toxic Chlorophenols

Mingyang Liu, Xuemei Yang and Paul J. Dyson*, *PNAS* **2022**, *119*, e2122425119
https://www.pnas.org/doi/epdf/10.1073/pnas.2122425119
Institute of Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Chlorophenols are persistent in herbicides, drugs and pesticides. They are slow to biodegrade resulting in prolonged exposure and environmental problems. At present aryl chlorides are extremely versatile synthetic precursors, yet benign chlorination techniques to prepare them remain underdeveloped. Herein the authors report the synthesis of aryl chlorides using chloro-group transfer from chlorophenol pollutants, during their destruction, to arene substrates. This results in valorisation of the chlorine atoms during the mineralization of the chlorophenol with a very high atom economy. A broad range of substrates that contain a range of different directing and functional groups could be transformed and a variety of different chlorophenol pollutants can be used as the chlorine source. It is hoped that this process will lead to the use of chlorophenols and other chemical waste in a similar manner.

Authors' comments:
Mingyang Liu (the first author) notes that, "chemists have created many valuable chemicals, but some have led to serious environmental problems. We have to ensure these chemicals could be decommissioned and destroyed in a sustainable manner."



Amplification of Light within Aerosol Particles Accelerates In-particle Photochemistry

Pablo Corral Arroyo, Grégory David, Peter A. Alpert, Eveleyne A. Parmentier, Markus Ammann, Ruth Signorell*, *Science* **2022**, *376*, 293–296
https://doi.org/10.1126/science.abm7915
ETH Zurich, Paul Scherrer Institute

The understanding of aerosol and cloud photochemistry is critical to evaluate the processing of atmospheric particulate matter and further improve global atmospheric models. Optical confinement (OC) effects amplify the light intensity within aerosol particles, and, theoretically, can accelerate photochemical reactions in micro- and nanodroplets. Herein, the authors report a novel investigation into the influence of OC in particle reactions. Using X-ray spectromicroscopic imaging, complemented with modelling, they found direct evidence for OC-induced composition patterning inside photoactive particles. Iron(III)-citrate particles were probed using the iron oxidation state as a photochemical marker. These results allowed the authors to predict an overall acceleration of photochemical reactions by a factor of two to three for most classes of atmospheric aerosol particles. Including this evidence in atmospheric aerosol and cloud models should allow improvement in global chemistry models and climate predictions.

Authors' comments:
"We show that OC effects accelerates significantly atmospheric photochemistry. This research will have a great impact on the atmospheric chemistry community. Global chemistry models need to be revised and updated."