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Swiss Science Concentrates

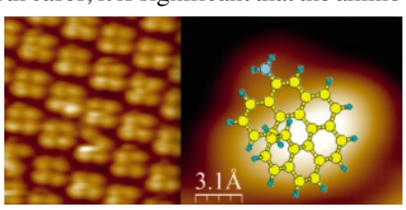
A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

Van der Waals Interactions in the Self-assembly of 5-Amino[6]helicene on Cu(100) and Au(111)

H. Ascolani*, M. W. van der Meijden, L. J. Cristina, J. E. Gayone, R. M. Kellogg, J. D. Fuhr*, and M. Lingenfelder*, *Chem. Commun.* **2014**, *50*, 13907. EPF Lausanne

The role of van der Waals interactions in the self-assembly of an aminohelicene on metal surfaces was elucidated using a combination of scanning tunnelling microscopy and density functional theory simulations. M. Lingenfelder and collaborators studied the self-assembly of 5-amino[6]helicene (AH) on copper and gold surfaces. While the C6 rings-surface interaction dominates in the case of Cu(100), the amino–surface interaction is crucial on Au(111). In both cases, it is significant that the amino group does not induce polar interactions *via* hydrogen bonding but rather that the maximization of vdW interactions drives the self-assembly.



Environmental and Economic Assessment of Lactic Acid Production from Glycerol Using Cascade Bio- and Chemocatalysis

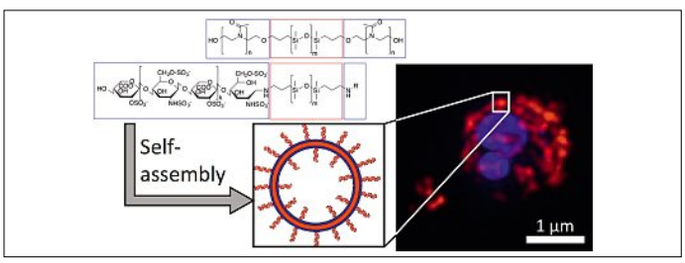
M. Morales, P. Y. Dapsens, I. Giovinazzo, J. Witte, C. Mondelli*, S. Papadokonstantakis*, K. Hungerbühler, and J. Pérez-Ramírez*, *Energy Environ. Sci.* **2015**, *8*, 558. ETH Zürich

Lactic acid (LA) has gained considerable interest as an intermediate in the conversion of bio-derived feedstocks into chemicals. LA is industrially prepared *via* anaerobic batch fermentation of glucose or sucrose and serves as a platform chemical with a large and rapidly expanding market. The authors introduce a novel cascade process comprising bio- and chemocatalytic steps to valorise glycerol obtained as a waste in the production of biodiesel by conversion into LA. Through the combination of catalyst design, process modelling and multi-criteria assessment, they demonstrate the advantages of this new route in terms of environmental footprint and profit compared to the currently practiced enzymatic technology.

Nanomimics of Host Cell Membranes Block Invasion and Expose Invasive Malaria Parasites

A. Najer, D. Wu, A. Bieri, F. Brand, C. G. Palivan, H.-P. Beck, and W. Meier*, *ACS Nano* **2014**, *8*, 12560. University of Basel

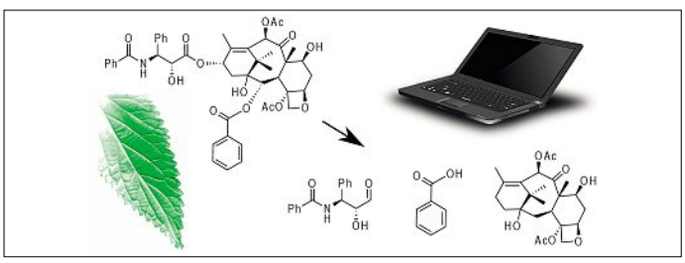
New drugs or vaccines against infectious diseases, such as malaria, are urgently needed. In an elegant approach, W. Meier and coworkers use polymersomes presenting receptors required for parasite attachment to host cells as stable nanomimics to efficiently interrupt the life cycle of *P. falciparum.* The nanomimics were shown to bind parasite-derived ligands involved in the initial attachment to host cells and thus blocking reinvasion of malaria parasites after egress from host cells *in vitro* was achieved. Additionally, this will expose the invasive form of the parasite to the immune system. This strategy might lead to a treatment option for severe malaria or an alternative way to modulate the immune response.



Revealing the Macromolecular Targets of Complex Natural Products

D. Reker, A. M. Perna, T. Rodrigues, P. Schneider, M. Reutlinger, B. Mönch, A. Koeberle, C. Lamers, M. Gabler, H. Steinmetz, R. Müller, M. Schubert-Zsilavecz, O. Werz, and G. Schneider*, *Nat. Chem.* **2014**, *6*, 1072. ETH Zürich

Even though natural products represent an invaluable source of pharmaceutically active compounds, their macromolecular targets are often unknown. G. Schneider and coworkers present the development and experimental validation of a computational method for the discovery of such targets. Their algorithm dissects the natural products into fragments and infers potential pharmacological targets by comparing the fragments to synthetic reference drugs with known targets. In a model study they demonstrate that fragments of the antitumor agent archazolid A contain relevant information regarding its polypharmacology. The results obtained corroborate the practical applicability of the computational approach to natural product 'de-orphaning'.



Prepared by Caroline D. Bösch, Markus Probst, Yuliia Vyborna, Mykhailo Vybornyi, Simon M. Langenegger and Robert Häner

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