

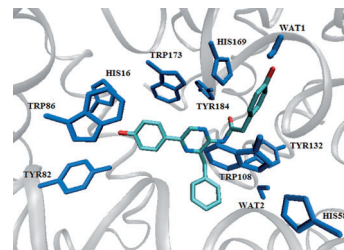


Computer Chemistry

S.-F. Chen, N. Ferré, Y.-J. Liu*

QM/MM Study on the Light Emitters of Aequorin
Chemiluminescence, Bioluminescence, and Fluorescence: A General Understanding of the Bioluminescence of Several Marine Organisms

See jellyfish in a new light: The origin and differences in the chemiluminescence, bioluminescence, and fluorescence of the proteins of the aequorin jellyfish were theoretically investigated by performing hybrid quantum mechanics and molecular mechanics methods combined with a molecular dynamics method. The findings are important for understanding the bioluminescence of jellyfish and other marine organisms (see figure).



Chem. Eur. J.
DOI: 10.1002/chem.201300678

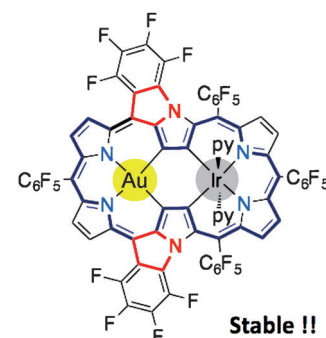


Hybrid Complexes

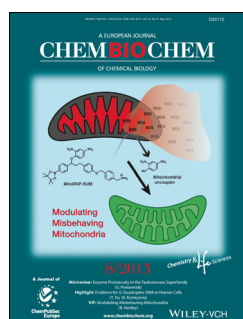
K. Naoda, H. Mori, A. Osuka*

Gold^{III}–Iridium^{III} Hybrid Complexes of Hexaphyrin(1.1.1.1.1.1)

Au revoloIR: Hexaphyrin Au^{III}–Ir^{III} complexes were prepared from the reaction of a mono-Au^{III} [26]hexaphyrin complex with [IrCl(cod)]₂ followed by treatment with pyridine. *N*-Fusion reaction of this complex gave a syn-doubly *N*-fused hexaphyrin as the major product, which displayed antiaromatic properties such as strong paratropic ring current, a small HOMO–LUMO gap and a low-energy forbidden absorption. The oxidation of this fused product with MnO₂ afforded an oxidatively cleaved product.



28 π Hückel Antiaromatic
Stable !!
Chem. Asian J.
DOI: 10.1002/asia.201300320

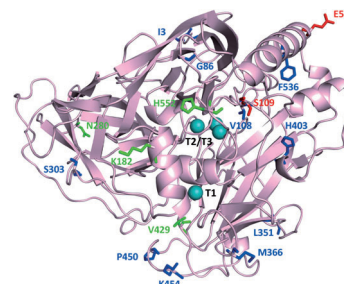


Directed Evolution

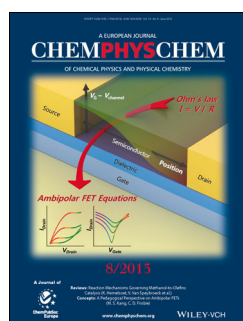
P. Torres-Salas, D. M. Mate, I. Ghazi, F. J. Plou, A. O. Ballesteros, M. Alcalde*

Widening the pH Activity Profile of a Fungal Laccase by Directed Evolution

Unnatural selection: A fungal laccase was tailored by directed evolution to be active at neutral/alkaline pH. After five generations, the final mutant showed a broader pH profile while retaining 50 to 80 % of its activity at neutral pH.



ChemBioChem
DOI: 10.1002/cbic.201300102

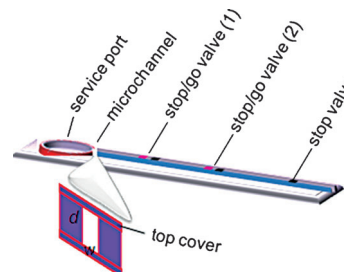


Carbon Electrodes

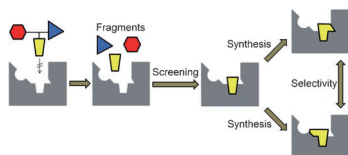
A. P. Washe, P. Lozano, D. Bejarano, I. Katakis*

Electrochemically Actuated Stop–Go Valves for Capillary Force-Operated Diagnostic Microsystems

Nanoporous graphitic carbon electrodes display a unique electrowetting behavior that depends on specific ion effects. When incorporated into a microfluidic channel, these superhydrophobic electrodes facilitate sequential stop–go fluidic operations, which are directly applicable to diagnostic microsystems.



ChemPhysChem
DOI: 10.1002/cphc.201300042



Subtype-Selective Ligands

A. J. Thompson, M. H. P. Verheij, J. E. van Muijlwijk-Koezen, S. C. R. Lummis,* R. Leurs, I. J. P. de Esch

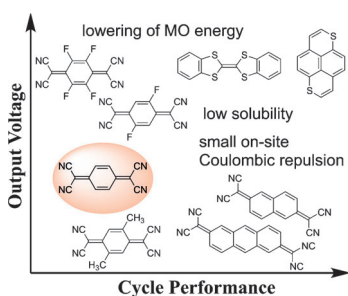
Structure–Activity Relationships of Quinoxaline-Based 5-HT₃A and 5-HT₃AB Receptor-Selective Ligands

One atom makes the difference: By using a fragment screen as an efficient route to design novel ligands, we identified quinoxalines as high-affinity binders to 5-HT₃ receptors. New synthesis routes allowed the development a series of compounds able to distinguish 5-HT₃A receptors from 5-HT₃AB receptors, revealing that a single atom is sufficient to change the selectivity profile of a compound.



ChemMedChem

DOI: 10.1002/cmdc.201300032

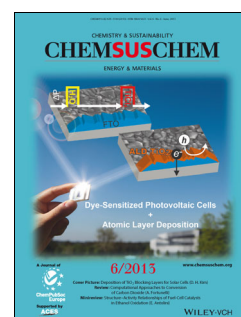


Batteries

S. Nishida, Y. Yamamoto, T. Takui,* Y. Morita*

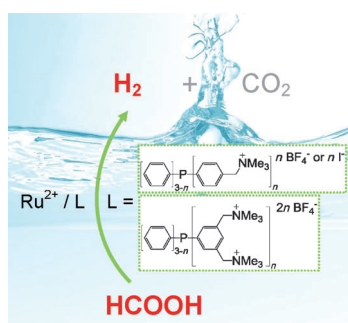
Organic Rechargeable Batteries with Tailored Voltage and Cycle Performance

Made to order: Rechargeable batteries are fabricated by using organic electron acceptors and donors as active cathode materials. Their output voltage and cycle performance can be tuned by organic chemistry techniques. The output voltages are linked to both the redox potentials and the energy levels of the frontier molecular orbitals of the cathode materials, enabling to predict the output voltage at an early stage of the design.



ChemSusChem

DOI: 10.1002/cssc.201300010

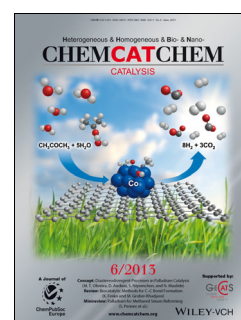


Oxidative Dehydrogenation

W. Gan, D. J. M. Snelders, P. J. Dyson, G. Laurenczy*

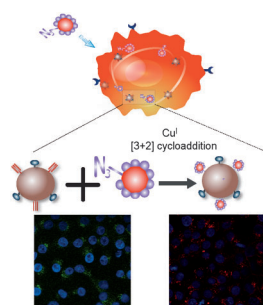
Ruthenium(II)-Catalyzed Hydrogen Generation from Formic Acid using Cationic, Ammoniomethyl-Substituted Triarylphosphine Ligands

Proceed with cation: New Ru^{II} catalysts for aqueous-phase HCOOH decomposition into H₂ and CO₂ that use a series of oligocationic, ammoniomethyl-substituted triarylphosphine ligands are developed. Excellent activities are achieved, that is, TOFs of 1950 h⁻¹ and TONs of over 10000.



ChemCatChem

DOI: 10.1002/cctc.201200782

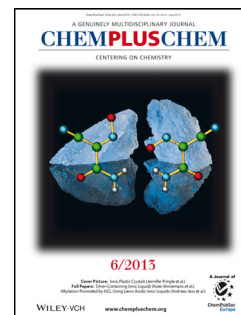


Tracking Multifunktional Nanoparticles

S. N. Goonewardena,* H. Zong, P. R. Leroueil, J. R. Baker, Jr.

Bioorthogonal Chemical Handle for Tracking Multifunctional Nanoparticles

Getting a handle on it: An innovative strategy for tracking multifunctional nanoparticles in biological systems is presented that simplifies the syntheses and can be used to track the nanoparticles in vitro and in vivo. The strategy is based on in situ click chemistry ligation of fluorescent reporters to the nanoparticle scaffold through copper-catalyzed azide–alkyne cycloaddition (see figure).



ChemPlusChem

DOI: 10.1002/cplu.201300007

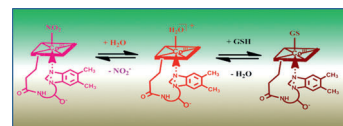


Cobalamins

D. T. Walker, R. S. Dassanayake, K. A. Garcia, R. Mukherjee, N. E. Brasch*

Mechanistic Studies on the Reaction of Nitrocobalamin with Glutathione: Kinetic Evidence for Formation of an Aquacobalamin Intermediate

Kinetic studies on the reaction of nitrocobalamin (NO_2Cbl) with glutathione show that glutathionylcobalamin (GSCbl) is formed via an aquacobalamin (H_2OCbl^+) intermediate. This reaction pathway is demonstrated by independently determining individual rate constants for each step.



Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201300254

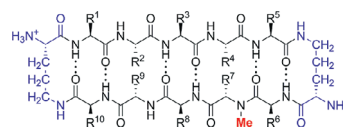


Macrocyclic β -Sheets

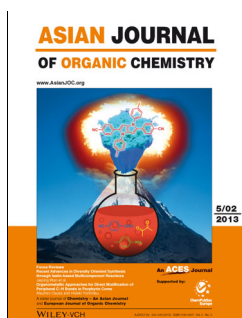
R. Spencer, K. H. Chen, G. Manuel, J. S. Nowick*

Recipe for β -Sheets: Foldamers Containing Amyloidogenic Peptide Sequences

Recipe for β -Sheets: Combine one *N*-methyl-amino acid, two δ -linked ornithine turn units, and nine α -amino acids by solid-phase peptide synthesis. Cyclize in solution, deprotect, and purify by RP-HPLC. Confirm folding by ^1H NMR ROESY and magnetic anisotropy studies. Serve to laboratories interested in studying and inhibiting amyloid aggregation or studying β -sheet assembly.



Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201300221

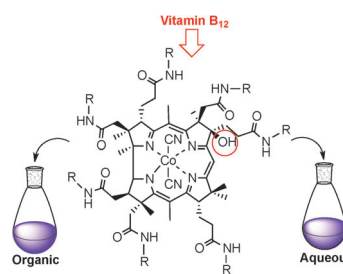


Cobyrinic Acid Derivatives

K. ó. Proinsias, M. Giedyk, Ł. Banach, D. Rutkowska-Zbik, D. Gryko*

Selectively Modified Cobyrinic Acid Derivatives

Vitamin B₁₂ - more possibilities: An efficient method for the aminolysis of cobyrinic acid derivatives catalyzed by a benzotriazole/DBU system is described. The synthesized cobinamide derivatives can be easily functionalized at either the *c* or *meso* position. $(\text{CN})_2\text{Cby}(\text{III})\text{OMe}$, is prone to hydroxylation at the C8 position. The location of hydroxylation was confirmed through NMR analysis and the reactivity of this position was analyzed by computational methods.



Asian J. Org. Chem.
DOI: 10.1002/ajoc.201300051

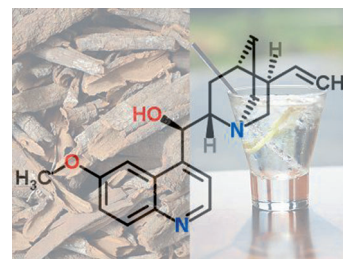


Quinine

K. Roth and S. Streller

From Pharmacy to the Pub - A Bark Conquers the World: Part 1

The bark of the Cinchona tree is probably the most valuable drug the Americas gave the world. It yielded the first effective remedy for malaria, one of the most dangerous of infectious diseases. Its main component, quinine, is still used as a medication - but also for tonic water and Bitter Lemon. K. Roth and S. Streller, Berlin, look at the history and, of course, chemistry of this important substance.



ChemViews magazine
DOI: 10.1002/chemv.201300056