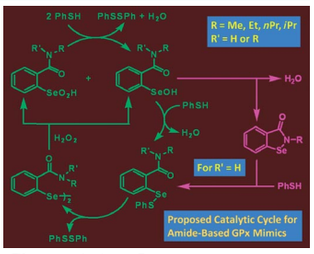
Enzyme Mimics

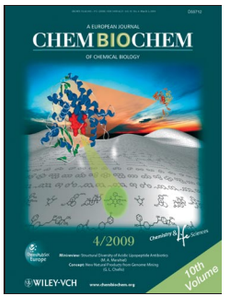
K. P. Bhabak, G. Mugesh*

Amide-Based Glutathione Peroxidase Mimics: Effect of Secondary and Tertiary Amide Substituents on Antioxidant Activity

Sec or terts: A series of *sec*- and *tert*-amide substituted diselenides have been synthesised as synthetic mimics of glutathione peroxidase (GPx), characterized, and studied for their antioxidant activities using H_2O_2, Cum-OOH, and *t*BuOOH as substrates and PhSH as thiol co-substrate. The substitution at the free –NH group of the amide moiety in the sec-amide based diselenides is shown to enhance the GPx activity.



Chem. Asian J.
DOI: **10.1002/asia.200800483**

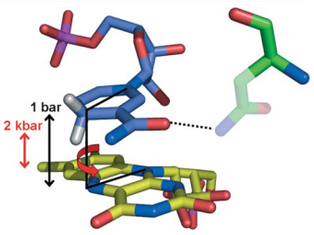


Catalysis

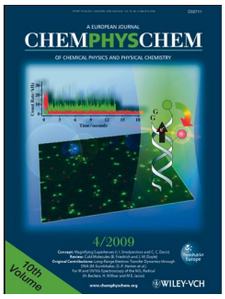
C. R. Pudney, T. McGrory, P. Lafite, J. Pang, S. Hay, D. Leys, M. J. Sutcliffe, N. S. Scrutton*

Parallel Pathways and Free-Energy Landscapes for Enzymatic Hydride Transfer Probed by Hydrostatic Pressure

Mutation of an active-site residue in morphinone reductase leads to a conformationally rich landscape that enhances the rate of hydride transfer from NADH to FMN at standard pressure (1 bar). Increasing the pressure causes interconversion between different conformational substates in the mutant enzyme. While high pressure reduces the donor–acceptor distance in the wild-type enzyme, increased conformational freedom "dampens" its effect in the mutant.



ChemBioChem
DOI: **10.1002/cbic.200900071**

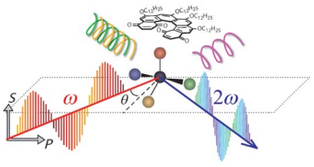


Chiral Spectroscopy

S. Foerier, I. A. Kolmychek, O. A. Aktsipetrov, T. Verbiest, V. K. Valev*

Optical Second Harmonic Generation Chiral Spectroscopy

Chiral spectroscopic study: The intensities of second harmonic generation chiral spectroscopy are obtained from the dispersion of the nonlinear optical susceptibility components, as a function of wavelength for helicenbisquinone thin films. A single formalism fits all the data simultaneously, and the findings constitute an important milestone towards the development of a new experimental technique.



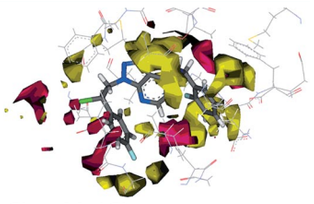
ChemPhysChem
DOI: **10.1002/cphc.200900045**

Molecular Modeling

F. Falchi, F. Manetti, F. Carraro, A. Naldini, G. Maga, E. Crespan, S. Schenone,* O. Bruno, C. Brullo, M. Botta*

3D QSAR Models Built on Structure-Based Alignments of Abl Tyrosine Kinase Inhibitors

Quality QSAR: A combination of docking calculations and a statistical approach toward Abl inhibitors resulted in a 3D QSAR model, the analysis of which led to the identification of ligand portions important for affinity. New compounds designed on the basis of the model were found to have very good affinity for the target, providing further validation of the model itself.



ChemMedChem
DOI: **10.1002/cmdc.200800441**

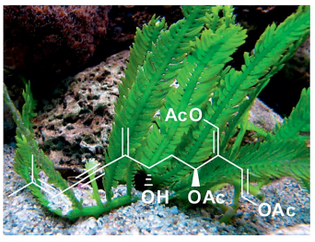
Angew. Chem. Int. Ed.
DOI: **10.1002/anie.200900755**

Click Chemistry

C. R. Becer, R. Hoogenboom, U. S. Schubert*

Click Chemistry beyond Metal-Catalyzed Cycloaddition

No copper needed: In recent years, a large number of metal-free click reactions have been reported based on thiol-ene radical additions, Diels–Alder reactions, and Michael additions. In this Minireview, special attention is given to the advantages and limitations of the different methods to evaluate whether they have the potential to surpass the overwhelming success of the copper(I)-catalyzed azide-alkyne cycloaddition.



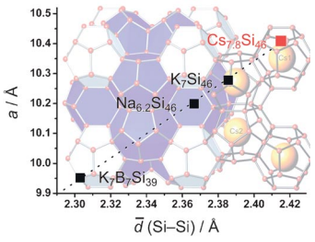
Eur. J. Org. Chem.
DOI: **10.1002/ejoc.200900101**

Toxic Sesquiterpenoids

L. Commeiras,* J. Thibonnet, J.-L. Parrain*

Studies towards the Total Synthesis of (–)-Caulerpenynol, a Toxic Sesquiterpenoid of the Green Seaweed *Caulerpa taxifolia*

The first diastereoselective synthesis of the antimicrobial and cytotoxic agent (–)-caulerpenynol (**2**) was achieved in relatively few steps from commercially available (*S*)-malic acid. Highlights of this synthesis include the nonracemization of the sensitive α-hydroxy ketone moiety and the correct choice of protecting groups for the critical last deprotection step.



Chem. Eur. J.
DOI: **10.1002/chem.200900307**

Clathrates

A. Wosylus, I. Veremchuk, W. Schnelle, M. Baitinger, U. Schwarz, Yu. Grin*

$Cs_{8-x}Si_{46}$: A Type-I Clathrate with Expanded Silicon Framework

The synthesis of the new binary $Cs_{8-x}Si_{46}$ (shown here) completes the series of binary alkali metal silicides with a clathrate-I structure $M_{8-x}Si_{46}$ (M = Na, K, Rb, Cs). In contrast to the lighter homologues, $Cs_{8-x}Si_{46}$ can be prepared only at elevated pressures. The compound was obtained at 1200 °C between 2–10 GPa and the Cs content rises with applied pressure.

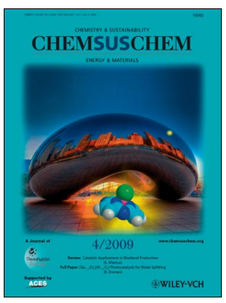
ChemSusChem
DOI: **10.1002/cssc.200900020**

Catalytic Oxidation

F. Cavani,* J. H. Teles

Sustainability in Catalytic Oxidation: An Alternative Approach or a Structural Evolution?

Catalytic oxidation provides several examples of the remarkable steps made forward towards a more sustainable chemical industry: use of alternative reactants, the design of new catalysts, new reactions, and new reactor technologies. The recent developments described in this Review clearly show that better sustainabily and improved economics often go hand in hand.



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