

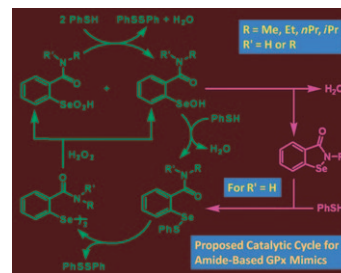


## Enzyme Mimics

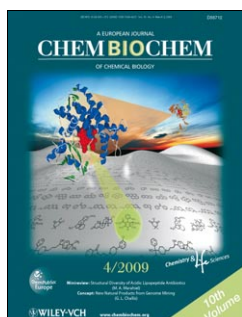
K. P. Bhabak, G. Mugesh\*

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

**Sec or tert:** 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

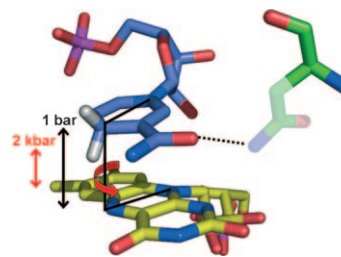


## Catalysis

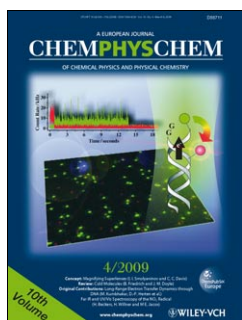
C. R. Pudney, T. McGrory, P. Lafite, J. Pang, S. Hay, D. Leys, M. J. Sutcliffe, N. S. Scrutton\*

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

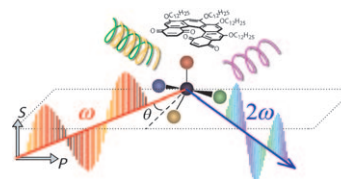


## Chiral Spectroscopy

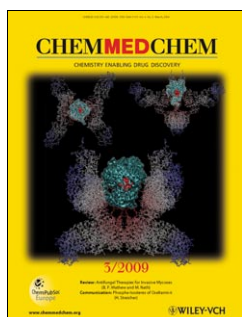
S. Foerier, I. A. Kolmychek, O. A. Aktsipetrov, T. Verbiest, V. K. Valev\*

Optical Second Harmonic Generation Chiral Spectroscopy

**Chiral spectroscopic study:** The intensities of second harmonic generation chiral spectroscopy are obtained from the dispersion of the non-linear 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

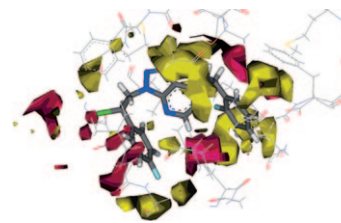


## Molecular Modeling

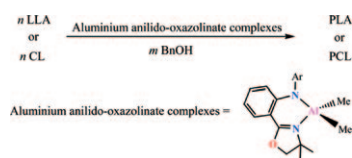
F. Falchi, F. Manetti, F. Carraro, A. Naldini, G. Maga, E. Crespan, S. Schenone,\* O. Bruno, C. Brullo, M. Botta\*

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



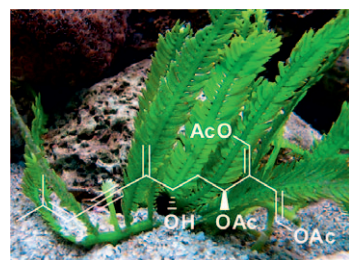
*Eur. J. Inorg. Chem.*  
DOI: 10.1002/ejic.200900064

## Ring-Opening Polymerization

C.-T. Chen,\* H.-J. Weng, M.-T. Chen, C.-A. Huang, K.-F. Peng

Synthesis, Characterization, and Catalytic Application of Aluminum Anilido-Oxazolinates Complexes

The aluminum complexes bearing anilido-oxazolinates ligands demonstrate efficient activities in catalyzing the ring-opening polymerization of L-lactide or  $\epsilon$ -caprolactone in the presence of benzyl alcohol.



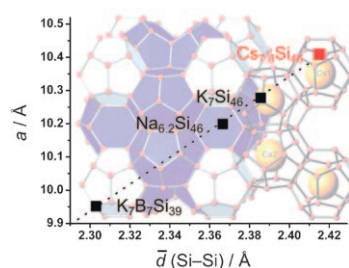
*Eur. J. Org. Chem.*  
DOI: 10.1002/ejoc.200900101

## 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  $\alpha$ -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\*

$\text{Cs}_{8-x}\text{Si}_{46}$ : A Type-I Clathrate with Expanded Silicon Framework

The synthesis of the new binary  $\text{Cs}_{8-x}\text{Si}_{46}$  (shown here) completes the series of binary alkali metal silicides with a clathrate-I structure  $\text{M}_{8-x}\text{Si}_{46}$  ( $\text{M} = \text{Na}, \text{K}, \text{Rb}, \text{Cs}$ ). In contrast to the lighter homologues,  $\text{Cs}_{8-x}\text{Si}_{46}$  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 sustainability and improved economics often go hand in hand.



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