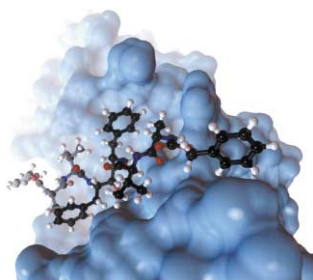


Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica



Cover

See A. Brik and C.-H. Wong, page 5.
The structure of FIV protease binding to the potent inhibitor TL-3 (image by G. M. Morris and A. J. Olson).



Chemical biology articles published in this journal also appear in the *Chemical Biology Virtual Journal*: www.rsc.org/chembiol

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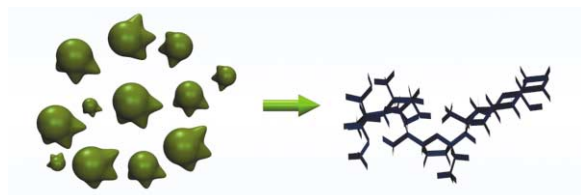


xi **Editorial:** Professor Ben Feringa

xii **Profile:** *Organic & Biomolecular Chemistry* profiles the Chair of the Editorial Board

EMERGING AREA

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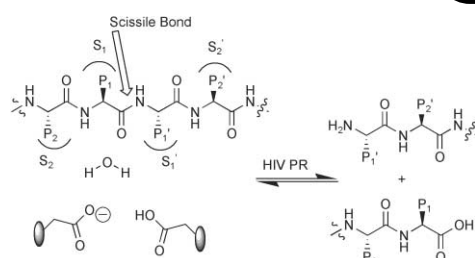
Metabolic engineering—a genetic toolbox for small molecule organic synthesis

Michael D. Burkart

Metabolic engineering is an emerging field in which genetic design regulates the enzymatic synthesis of small molecules *in vivo*.

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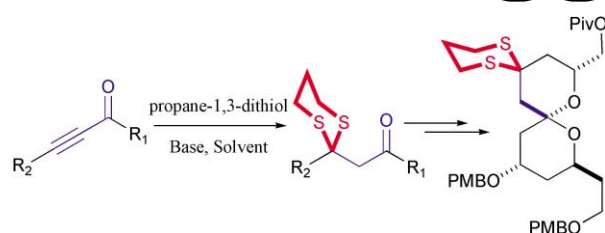
**HIV-1 protease: mechanism and drug discovery**

Ashraf Brik and Chi-Huey Wong

Studies conducted on the mechanism of HIV PR and the impact of their conclusions on drug discovery processes.

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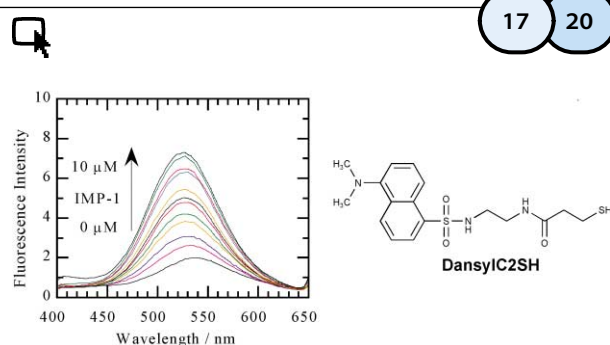
**Development of β -keto 1,3-dithianes as versatile intermediates for organic synthesis**

Matthew J. Gaunt, Helen F. Sneddon, Peter R. Hewitt, Paolo Orsini, David F. Hook and Steven V. Ley

Dithiol additions to propargylic carbonyl compounds provide a versatile platform for the synthesis of 1,3-oxygenated molecules.

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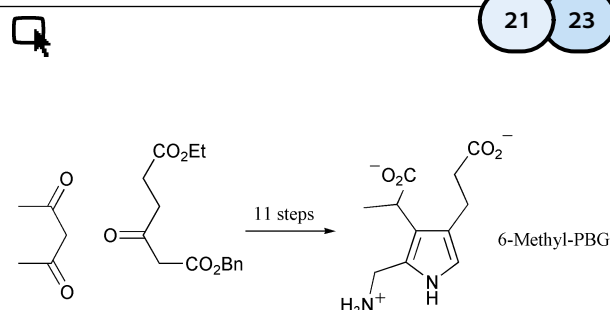
**Detection of a metallo- β -lactamase (IMP-1) by fluorescent probes having dansyl and thiol groups**

Hiromasa Kurosaki, Hisami Yasuzawa, Yoshihiro Yamaguchi, Wanchun Jin, Yoshichika Arakawa and Masafumi Goto

The DansylC2SH, fluorescent probe, was found to yield increased fluorescence by binding with a metallo- β -lactamase (IMP-1).

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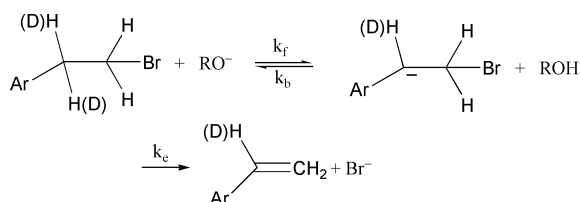
**A new synthesis of porphobilinogen analogues, inhibitors of hydroxymethylbilane synthase**

Raef Ahmed and Finian J. Leeper

6-Methyl-PBG is the most potent inhibitor of hydroxymethylbilane synthase (PBG deaminase) yet reported, with $K_i = 3 \mu$ M.

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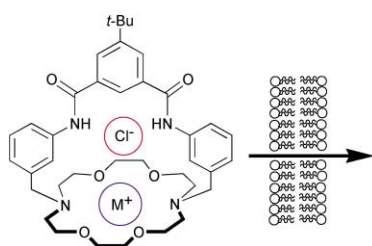
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**Resolution of the non-steady-state kinetics of the elimination of HBr from 2-(*p*-nitrophenyl)ethyl bromide in alcohol/alkoxide media**

Kishan L. Handoo, Yun Lu, Yixing Zhao and Vernon D. Parker

A classical concerted E2 reaction is shown actually to occur *via* a two-step mechanism.

27 29

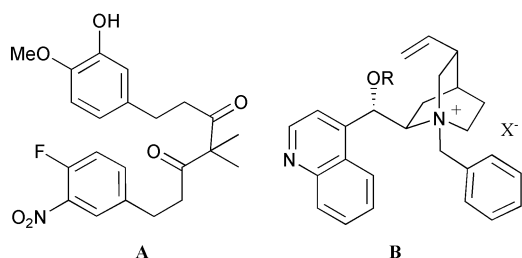


Facilitated transport of sodium or potassium chloride across vesicle membranes using a ditopic salt-binding macrobicyclic

Atanas V. Koulov, Joseph M. Mahoney and Bradley D. Smith

A synthetic receptor able to bind sodium or potassium chloride as a contact ion-pair can transport either salt across a vesicle membrane effectively.

30 32

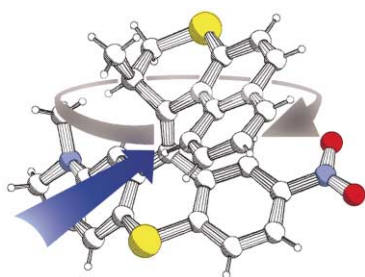


From central to planar chirality, the first example of atropenantioselective cycloetherification

Gabriela Islas-Gonzalez, Michèle Bois-Choussy and Jieping Zhu

Atropenantioselective cycloetherification of linear achiral diarylheptanoid (**A**) promoted by chiral base (**B**) is reported.

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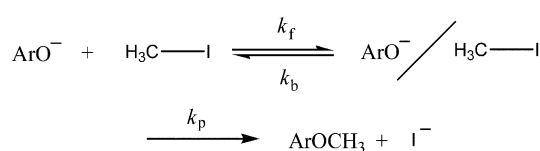


A donor-acceptor substituted molecular motor: unidirectional rotation driven by visible light

Richard A. van Delden, Nagatoshi Koumura, Annemarie Schoevaars, Auke Meetsma and Ben L. Feringa

A donor-acceptor substituted molecular motor allows visible light driven unidirectional rotation.

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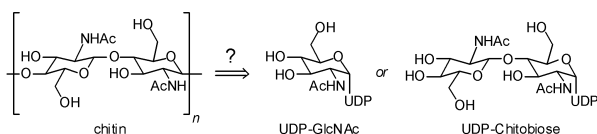


Non-steady-state kinetic study of the S_N2 reaction between *p*-nitrophenoxide ion and methyl iodide in aprotic solvents containing water. Evidence for a 2-step mechanism

Yun Lu, Kishan L. Handoo and Vernon D. Parker

A two-step mechanism for the S_N2 reaction between *p*-nitrophenoxide ion and methyl iodide in aprotic solvents containing water is presented.

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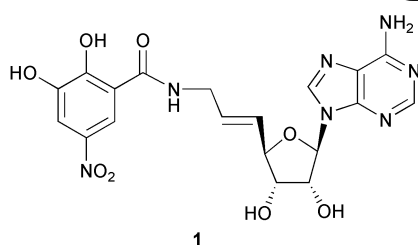
Probing the mechanism of a fungal glycosyltransferase essential for cell wall biosynthesis. UDP-Chitobiose is not a substrate for chitin synthase

Robert Chang, Adam R. Yeager and Nathaniel S. Finney

Is chitin biosynthesized from the minimum chemical or the minimum structural repeat unit?

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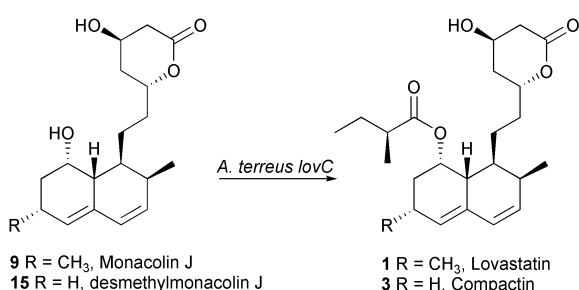
Bisubstrate inhibitors for the enzyme catechol-*O*-methyltransferase (COMT): influence of inhibitor preorganisation and linker length between the two substrate moieties on binding affinity

Christian Lerner, Birgit Masjost, Armin Ruf, Volker Gramlich, Roland Jakob-Roetne, Gerhard Zürcher, Edilio Borroni and François Diederich

The affinity of bisubstrate inhibitors *in vitro* for catechol *O*-methyltransferase is both dependent on inhibitor preorganisation and the length of the linker between nucleoside and catechol moieties.

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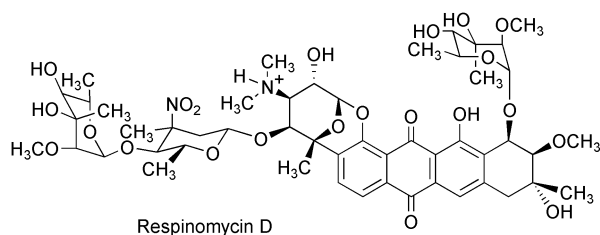
Transformations of cyclic nonaketides by *Aspergillus terreus* mutants blocked for lovastatin biosynthesis at the *lovA* and *lovC* genes

John L. Sorensen, Karine Auclair, Jonathan Kennedy, C. Richard Hutchinson and John C. Vederas

A marked difference in the nonaketide transforming abilities of *Aspergillus terreus lovA* and *lovC* disruptants

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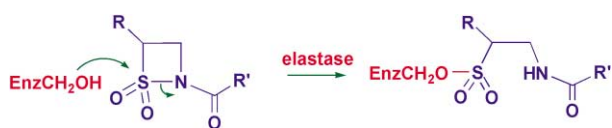
DNA recognition by the anthracycline antibiotic respinomycin D: NMR structure of the intercalation complex with d(AGACGTCT)₂

Mark S. Searle, Allister J. Maynard and Huw E. L. Williams

High resolution NMR data and molecular dynamics simulations have enabled the solution structure of the DNA intercalation complex of respinomycin D to be determined to investigate the role of sugar residues in DNA binding and recognition.

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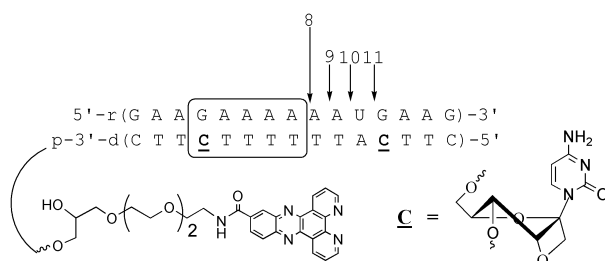
Structure–reactivity relationships in the inactivation of elastase by β-sultams

Paul S. Hinchliffe, J. Matthew Wood, Andrew M. Davis, Rupert P. Austin, R. Paul Beckett and Michael I. Page

The rate of inactivation of elastase by β-sultams is shown to be dependent on the nature of substituents on the sultam.

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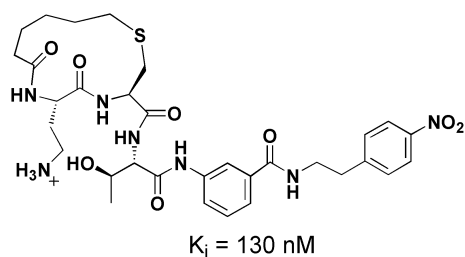
Antisense oligonucleotides with oxetane-constrained cytidine enhance heteroduplex stability, and elicit satisfactory RNase H response as well as showing improved resistance to both exo and endonucleases

Pushpangadan, I. Pradeepkumar, Nariman V. Amirkhanov and Jyoti Chattopadhyaya

Oxetane-constrained cytidine-incorporated antisense oligonucleotides as potential antisense candidates with fully phosphate backbones for further biological assessment.

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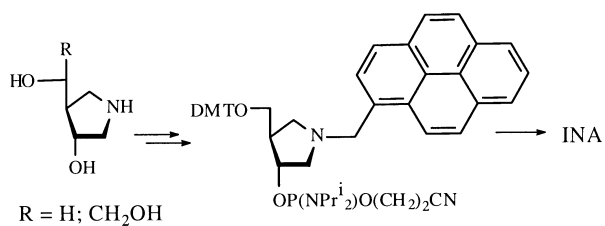
Peptides to peptidomimetics: towards the design and synthesis of bioavailable inhibitors of oligosaccharyl transferase

Eranthie Weerapana and Barbara Imperiali

Peptidomimetic inhibitors of oligosaccharyl transferase, the enzyme responsible for *N*-linked glycosylation, have been systematically developed.

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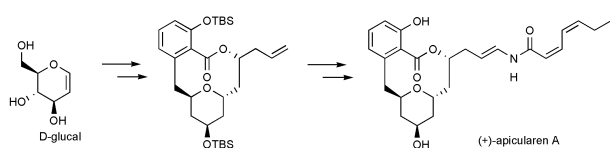
Intercalating nucleic acids (INAs) with insertion of *N*-(pyren-1-ylmethyl)-(3*R*,4*R*)-4-(hydroxymethyl)pyrrolidin-3-ol. DNA (RNA) duplex and DNA three-way junction stabilities

Vyacheslav V. Filichev and Erik B. Pedersen

Several intercalating nucleic acids have been synthesised and their discrimination between ssDNA and ssRNA investigated. These findings will be helpful in molecular design of targets and probes for DNA diagnostics.

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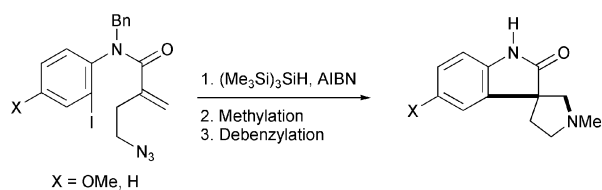
A formal total synthesis of (+)-apicularen A: base-induced conversion of apicularen-derived intermediates into salicylilhalamide-like products

Arwel Lewis, Ian Stefanuti, Simon A. Swain, Stephen A. Smith and Richard J. K. Taylor

The formal total synthesis of (+)-apicularen A is described.

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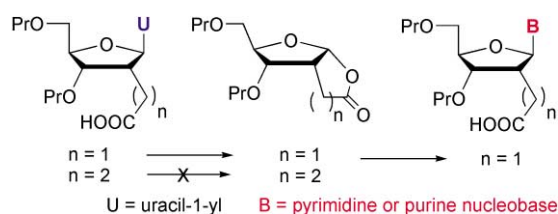
Concise synthesis of (±)-horsfiline and (±)-coerulecine by tandem cyclisation of iodoaryl alkenyl azides

Dimitrios E. Lizos and John A. Murphy

In the pursuit of candidates for antitumour testing, a rapid route to horsfiline and coerulecine is achieved by iodoaryl alkenyl azide tandem radical cyclisation reaction.

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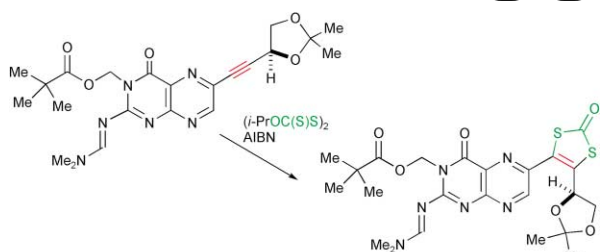


Studies on 2'- α -C-carboxyalkyl nucleosides and their application to a stereocontrolled nucleobase exchange process

Volker Fehring, Sally Knights, Mai-Yee Chan, Ian A. O'Neil and Richard Cosstick

Protected 2'- α -C-(carboxymethyl)uridine undergoes a two-step, stereocontrolled, nucleobase exchange process.

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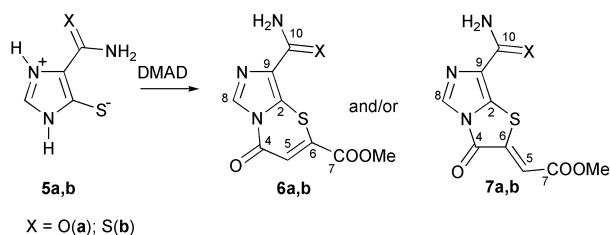


Synthesis of 1,3-dithiol-2-ones as proligands related to molybdopterin

Ben Bradshaw, David Collison, C. David Garner and John A. Joule

Creation of 4,5-disubstituted 1,3-dithiol-2-ones from disubstituted alkynes and diisopropyl xanthogen disulfide.

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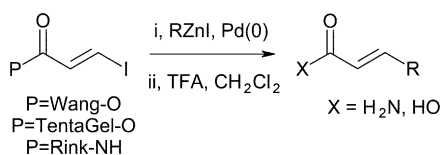


Reactions of 5-mercaptoazoles and pyridine-2-thiones with acetylenic esters. Selectivity of the formation of novel fused thiazin-4-ones and thiazolidin-4-ones

Vasiliy A. Bakulev, Vera S. Berseneva, Natalia P. Belskaia, Yury Yu. Morzherin, Andreiy Zaitsev, Wim Dehaen, Ingrid Luyten and Suzanne Toppet

The reactions of dimethyl acetylenedicarboxylate (DMAD) and methyl propynoate with 5-mercaptoazoles and pyridine-2-thiones lead to the selective formation of fused heterocyclic compounds.

140 144

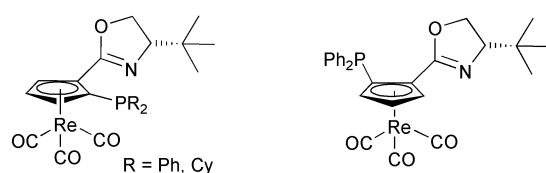


Cross coupling reactions of organozinc iodides with solid-supported electrophiles: synthesis of 4-substituted benzoic and 3-substituted (*E*)- and (*Z*)-propenoic acids and amides

Leslie J. Oates, Richard F. W. Jackson and Michael H. Block

Preparation of (*E*)- and (*Z*)-3-substituted propenoic acid derivatives can be achieved by coupling of organozinc reagents to solid-supported iodopropenoic acid.

145 152

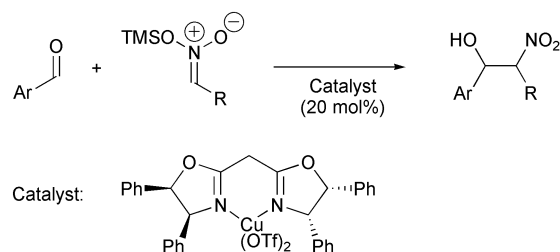


Synthesis of novel chiral phosphinocyrhetryloxazoline ligands and their application in asymmetric catalysis

Carsten Bolm, Li Xiao and Martin Kesselgruber

Cyrhetrynes prove to be a new family of ligands with promising properties in asymmetric catalytic reactions.

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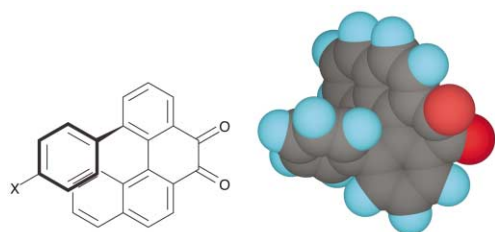


Catalytic asymmetric Henry reactions of silyl nitronates with aldehydes

Tine Risgaard, Kurt V. Gothelf and Karl Anker Jørgensen

The first catalytic asymmetric Henry reaction of silyl nitronates with aldehydes has been developed by trapping unstable nitroaldols using (*S*)-MTPA-Cl to form the corresponding Mosher esters.

157 162

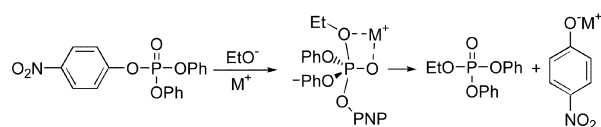


Through-space interactions between face-to-face, center-to-edge oriented arenes: importance of polar- π effects

Franco Cozzi, Rita Annunziata, Maurizio Benaglia, Mauro Cinquini, Laura Raimondi, Kim K. Baldrige and Jay S. Siegel

Through-space interactions between parallel offset arenes are dominated by electrostatic effects.

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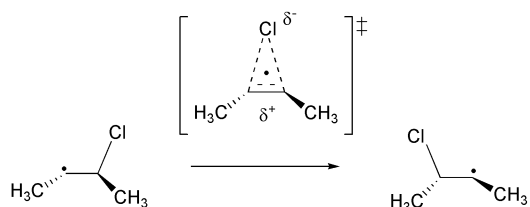


Alkali-metal ion catalysis and inhibition in nucleophilic displacement reactions at carbon, phosphorus and sulfur centres. IX. *p*-Nitrophenyl diphenyl phosphate

Ruby Nagelkerke, Gregory R. J. Thatcher and Erwin Buncel

Studies on alkali-metal ion catalysis and inhibition in nucleophilic displacement reactions at carbon, phosphorus and sulfur centres: catalytic activity of M⁺ follows the order Li⁺ > Na⁺ > K⁺ > Cs⁺.

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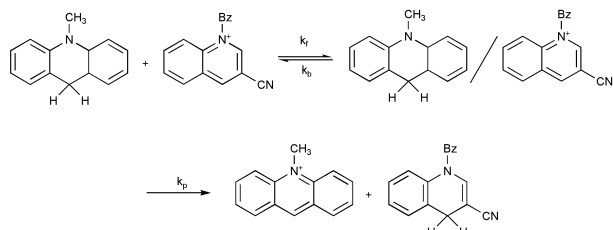


1,2-Chlorine atom migration in 3-chloro-2-butyl radicals: a computational study

Bernd Neumann and Hendrik Zipse

Skell's hypothesis of bridged 2-haloalkyl radicals has been revisited using several different theoretical methods and the 3-chloro-2-butyl radical as an example.

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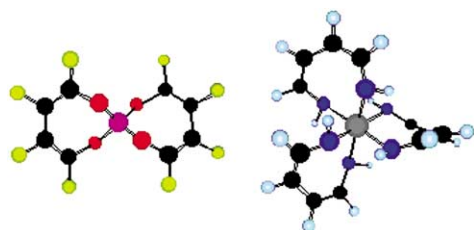


Hydride-exchange reactions between NADH and NAD⁺ model compounds under non-steady-state conditions. Apparent and real kinetic isotope effects

Yun Lu, Yixing Zhao, Kishan L. Handoo and Vernon D. Parker

The hydride transfer reaction in acetonitrile was observed to follow the 2-step mechanism accompanied by extensive hydride tunneling.

182 185

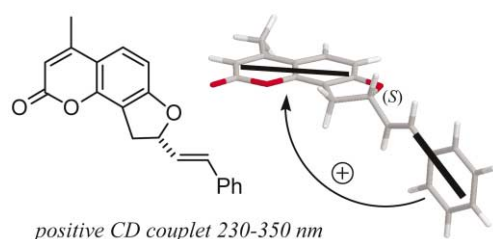


Möbius bis and tris-spiroaromatic systems

David Hall and Henry S. Rzepa

A series of 4- and 6-coordinate systems containing a main group atom (X) which can act as a spiroaromatic bridge across two aromatic ring systems are studied. As components of the bis-spiro rings **2** the effect is to create mildly Möbius-aromatic rings and the aromaticity is enhanced by ring fluorination, and by the nature of X.

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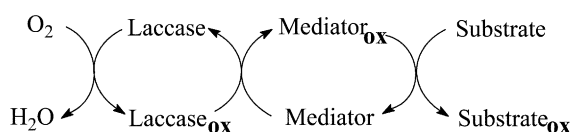


Assignment of absolute configuration of a chiral phenyl-substituted dihydrofuroangelicin

Gennaro Pescitelli, Nina Berova, Tom L. Xiao, Roman V. Rozhkov, Richard C. Larock and Daniel W. Armstrong

A synthetic coumarin derivative was resolved by chiral HPLC and its absolute configuration assigned by non-empirical CD analysis.

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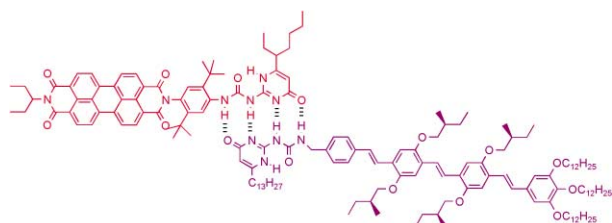


Promoting laccase activity towards non-phenolic substrates: a mechanistic investigation with some laccase–mediator systems

Paola Baiocco, Anna Maria Barreca, Maura Fabbrini, Carlo Galli and Patrizia Gentili

Fundamental reactivity features of the mediation phenomenon with the enzyme laccase towards non-phenolic substrates, and a comprehensive mechanistic rationalisation of it.

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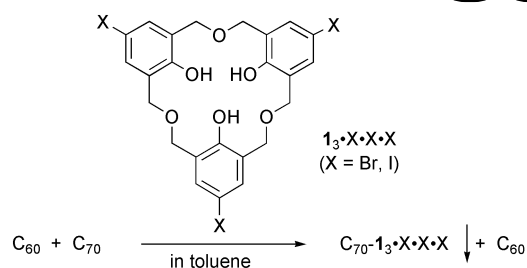


Singlet-energy transfer in quadruple hydrogen-bonded oligo(*p*-phenylenevinylene)perylene-diimide dyads

Edda E. Neuteboom, Edwin H. A. Beckers, Stefan C. J. Meskers, E. W. Meijer and René A. J. Janssen

Singlet-energy transfer in a quadruple hydrogen bonded supramolecular donor–acceptor dyad occurs within ~5 ps as inferred from transient spectroscopy.

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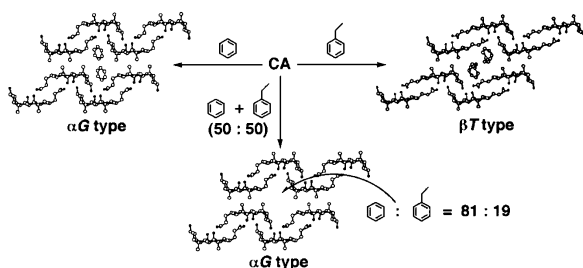


Preferential precipitation of C₇₀ over C₆₀ with *p*-halohomooxalix[3]arenes

Naoki Komatsu

C₇₀ is preferentially precipitated from a toluene solution of C₆₀ and C₇₀ with *p*-trihalohomooxalix[3]arenes.

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Dependence of selective enclathration on types of cholic acid crystals

Nungruethai Yoswathananont, Kazuki Sada, Mikiji Miyata, Shigendo Akita and Kazunori Nakano

Competitive recrystallizations of cholic acid from 1 : 1 binary mixtures of mono-substituted benzenes afford bilayer type inclusion crystals.

INSTRUCTIONS FOR AUTHORS

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Dates, venues and contact details of forthcoming events.

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