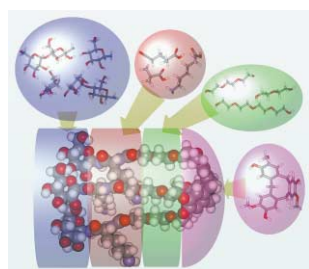


Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica

**Cover**

See J. van Ameijde and R. M. J. Liskamp, page 2661.

The cover picture illustrates the modular construction of a representative member from a library of trivalent amino acid glycoconjugate molecular constructs based on the cyclotrimeratrylene ('CTV') scaffold. The CTV scaffold (right) is capable of orienting in parallel three biofunctional arms composed of building blocks derived from pools of carbohydrates, amino acids and oligoethylene glycol spacers. The modular synthesis holds promise for the construction of libraries of other diverse molecules to be used for studying of or interference with a variety of biomolecular interactions.



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contents

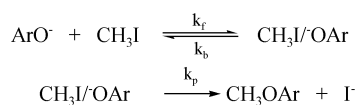
COMMUNICATIONS

2621 2623

Non-steady-state kinetic study of the S_N2 reaction between *p*-nitrophenoxide ion and methyl iodide in acetonitrile

Vernon D. Parker and Yun Lu

The S_N2 reaction between *p*-nitrophenoxide ion and methyl iodide takes place by a 2-step mechanism involving an intermediate reactant complex.

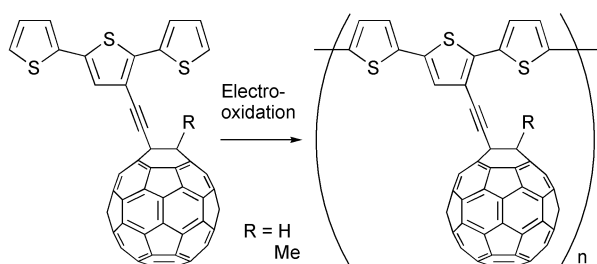


2624 2625

Synthesis and electropolymerization of fullerene-terthiophene dyads

Yasujiro Murata, Mitsuharu Suzuki and Koichi Komatsu

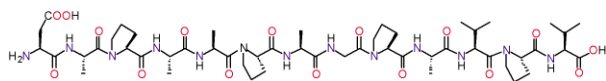
The first fullerene-terthiophene dyads were synthesized and their electropolymerization was shown to give electroactive polymer films.



2626 2629

Effects of β -sheet breaker peptide polymers on scrapie-infected mouse neuroblastoma cells and their affinities to prion protein fragment PrP(81–145)

Takehisa Oishi, Ken-ichi Hagiwara, Tomoya Kinumi, Yoshio Yamakawa, Masahiro Nishijima, Kazuhiko Nakamura and Hirokazu Arimoto

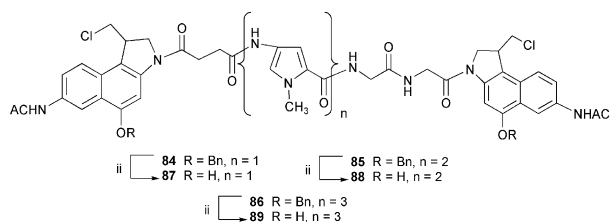
The direct binding of i-PrP13 might not play a major role in the inhibition of PrP^{Sc} formation.

ARTICLES

2630 2647

Synthesis and cytotoxicity evaluation of novel C7–C7, C7–N3 and N3–N3 dimers of 1-chloromethyl-5-hydroxy-1,2-dihydro-3H-benzo[e]indole (*seco*-CBI) with pyrrole and imidazole polyamide conjugates

Rohtash Kumar and J. William Lown

The C7–C7, C7–N3 and N3–N3 dimers of 1-chloromethyl-5-hydroxy-1,2-dihydro-3H-benzo[e]indole (*seco*-CBI) with pyrrole and imidazole polyamides were synthesized and preliminary anti-cancer evaluation carried out by NCI against three types of cancer cells.

2648 2654

The HLA-A2-supermotif: a QSAR definition

Irina Doytchinova and Darren Flower

We have developed a partial least squares based robust multivariate statistical method for the quantitative prediction of peptide binding to major histocompatibility complexes (MHC), the principal checkpoint on the antigen presentation pathway.

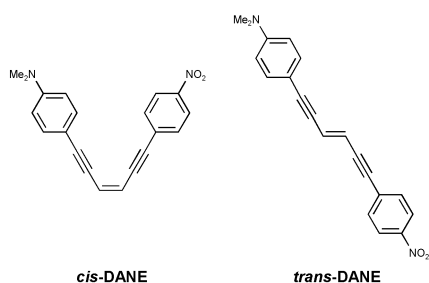


Preferred	F	I	G	I	L	I	F	V
	1	2	3	4	5	6	7	8
Deleterious		T		W	S		D	A

2655 2660

The photochemical characteristics of aromatic enediyne compounds substituted with electron donating and electron withdrawing groups

Yoshihiro Miki, Atsuya Momotake and Tatsuo Arai

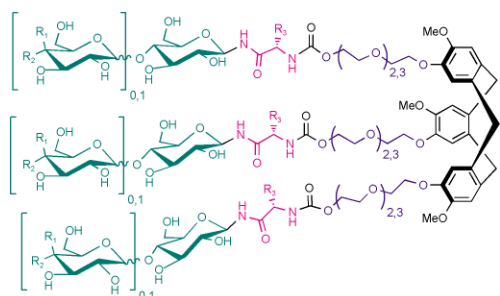
Small changes of solvent polarity in the less-polar region affected the fluorescence properties of *trans*-DANE due to the introduction of “push–pull” substituents.

2661 2669

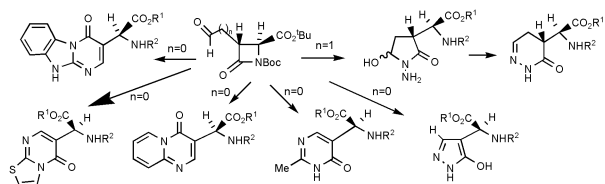
Synthesis of novel trivalent amino acid glycoconjugates based on the cyclotrimeratrylene (‘CTV’) scaffold

Jeroen van Ameijde and Rob M. J. Liskamp

Cyclotrimeratrylene (‘CTV’) as a versatile trivalent scaffold for attachment of a diversity of biomolecules: amino acid and carbohydrate residues.



2670 2681

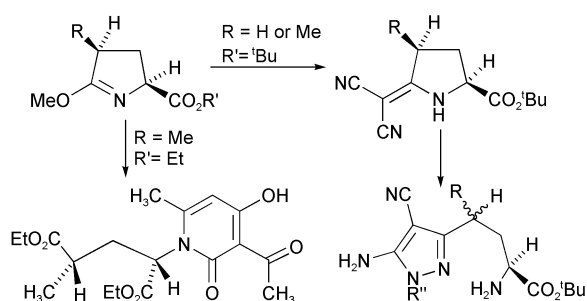


β -Lactams as versatile synthons for homochiral ibotenate analogues with potential for activity at glutamate receptors

Peter B. Hitchcock, Konstantinos Papadopoulos and Douglas W. Young

Activated aldehydes, $n = 0$ and 1 were synthesised and used to prepare homochiral heterocyclic analogues of ibotenic acid as shown.

2682 2688

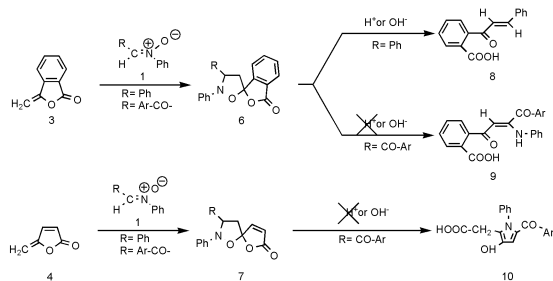


An alternative to the use of δ -lactam urethanes in the “ring switch” approach to higher homologues of AMPA-type glutamate antagonists

Peter B. Hitchcock, Shazia Rahman (née Masood) and Douglas W. Young

5-Exomethylene derivatives of pyroglutamate esters can be used to prepare homochiral homologues of AMPA antagonists.

2689 2698

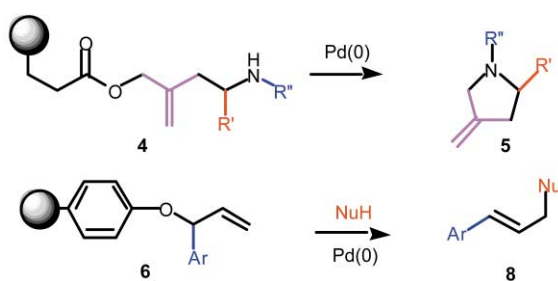


Spiroheterocycles from reaction of nitrones with methylene- γ -butyrolactones and some of their rearrangements

Christophe Roussel, Rachid Fihi, Kabula Ciamala, Joël Vebrel, Touria Zair and Claude Riche

All spiroadducts were formed *via* a very high regioselectivity pathway, the spirocarbon atom being linked to the isoxazolidine oxygen atom. Treatment of the spiroadducts in acidic and alkaline media led to unexpected and novel rearrangements.

2699 2709

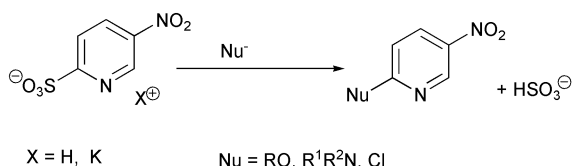


Solid-phase synthesis of 4-methylene pyrrolidines and allylic amines using palladium-activated allylic linkers

Richard C. D. Brown, Martyn L. Fisher and Lynda J. Brown

The synthesis of 4-methylene pyrrolidines and 3-aryl-allylamines has been achieved by palladium-catalysed nucleophilic cleavage of allylic ester and allylic ether linkages.

2710 2715

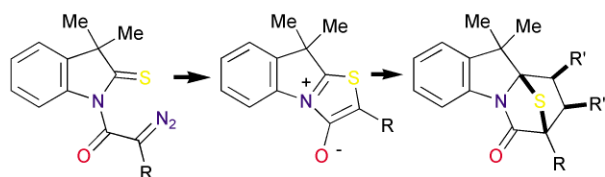


Substitution reactions of 5-nitropyridine-2-sulfonic acid. A new pathway to 2,5-disubstituted pyridines

Jan M. Bakke and Ingrid Sletvold

Substitution reactions of 5-nitropyridine-2-sulfonic acid are described whereby a variety of 2-substituted 5-nitropyridine compounds have been readily prepared, including 2-alkoxy-, 2-amino-, 2-alkyl and 2-chloro-5-nitropyridine in high yield.

2716 2722

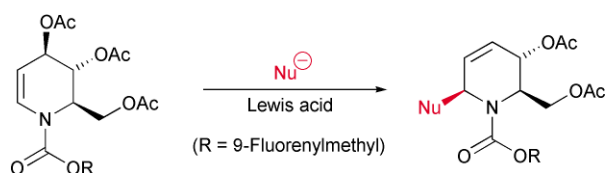


Dirhodium(II) tetraacetate catalysed reactions of diazo thioamides: isolation and cycloaddition of anhydro-4-hydroxy-1,3-thiazolium hydroxides (thioisomünchnones), an approach to analogues of dehydrogliotoxin

Christopher J. Moody, Alexandra M. Z. Slawin and David Willows

Dirhodium(II) catalysed reaction of indoline diazo thioamide gives stable thioisomünchnones; the masked thiocarbonyl ylide readily undergoes 1,3-dipolar cycloaddition.

2723 2733

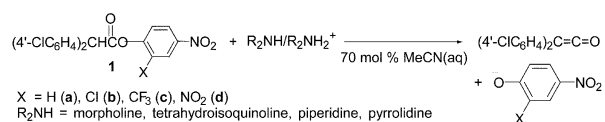


Preparation and reactivity of imino glycols: stereocontrolled, divergent approach to imino sugars

Paul J. Dransfield, Paul M. Gore, Ivan Prokeš, Michael Shipman and Alexandra M. Z. Slawin

Imino glycols undergo stereocontrolled Lewis acid mediated carbon-carbon bond forming reactions by allylic displacement of the C-3 acetate group.

2734 2738

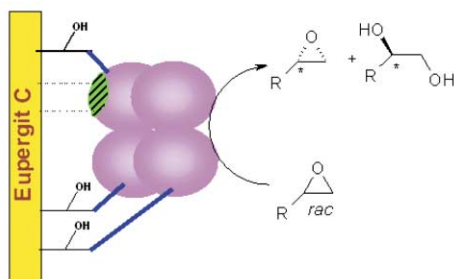


Ketene-forming eliminations from aryl bis(4'-chlorophenyl)acetates promoted by R₂NH-R₂NH₂⁺ in aqueous MeCN. Change of mechanism

Sang Yong Pyun, Dong Choon Lee, Ju Chang Kim and Bong Rae Cho

The mechanism of elimination from (4'-ClC₆H₄)₂CHCO₂C₆H₃-2-X-4-NO₂ promoted by R₂NH-R₂NH₂⁺ in aqueous MeCN changes from E2 to a concurrent E2 and E1cb by a poor leaving group.

2739 2743

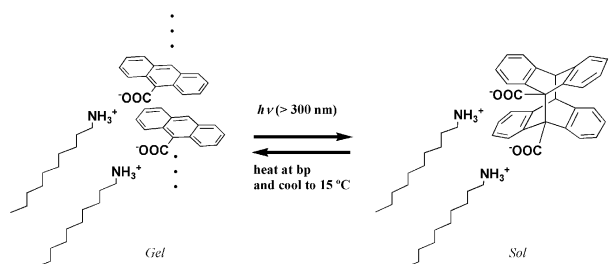


Enzymatic transformations. Immobilized *A. niger* epoxide hydrolase as a novel biocatalytic tool for repeated-batch hydrolytic kinetic resolution of epoxides

Cesar Mateo, Alain Archelas, Roberto Fernandez-Lafuente, Jose Manuel Guisan and Roland Furstoss

Efficient covalent immobilisation of the *A. niger* epoxide hydrolase is described, allowing the "repeated batch" kinetic resolution of epoxides.

2744 2747



Binary organogelators which show light and temperature responsiveness

Masatsugu Ayabe, Takanori Kishida, Norifumi Fujita, Kazuki Sada and Seiji Shinkai

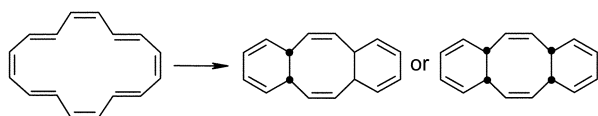
A cyclohexane gel of alkyllammonium anthracene-9-carboxylate shows reversible sol-gel phase transition events upon photodimerization and thermal isomerization of the anthracene moieties.



2748 2754

Computational study on the electrocyclic reactions of [16]annulene

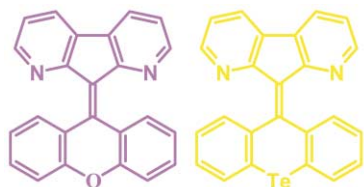
Ho-Lam Lee and Wai-Kee Li

Ab initio and DFT methods have been employed to study the electrocyclic reactions of [16]annulene.

2755 2763

Overcrowded 1,8-diazafluorenylidene-chalcoxanthenes. Introducing nitrogens at the fjord regions of bistricyclic aromatic enes

Amalia Levy, Shmuel Cohen and Israel Agranat

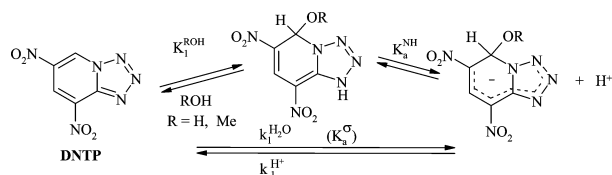
The effects of introducing nitrogen atoms in the fjord regions and chalcogen bridges on the conformations of overcrowded bistricyclic aromatic enes have been studied by ^1H , ^{13}C , ^{77}Se and ^{125}Te NMR spectroscopy and by X-ray analysis.

2764 2770

An extremely highly electrophilic heteroaromatic structure: 4,6-dinitrotetrazolo[1,5-*a*]pyridine

Taoufik Boubaker, Régis Goumont, Emmanuel Jan and François Terrier

Rate and equilibrium data for water and methanol addition to DNTP emphasize the superelectrophilic character of this neutral heterocycle.

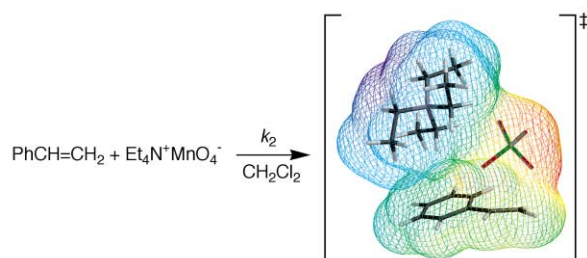


2771 2776

An experimental and theoretical study on the substituent effect of the permanganate oxidation of styrenes

Toshio Ogino, Hisashi Yaezawa, Osamu Yoshida and Mayumi Ono

Kinetic data obtained for the permanganate oxidation of alkenes are analysed by the semi-quantitative FMO treatment and DFT calculations of activation parameters based on the [3 + 2] transition model.

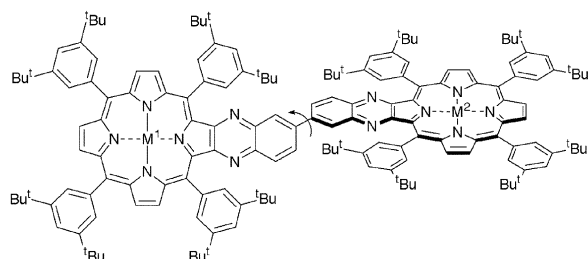


2777 2787

Synthesis and physical properties of biquinoxalinylyl bridged bis-porphyrins: models for aspects of Photosynthetic Reaction Centres

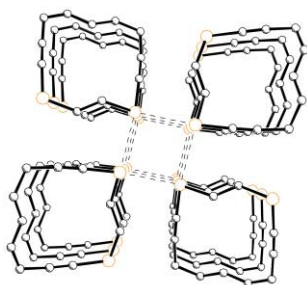
Maxwell J. Crossley, Paul J. Santic, Robin Walton and Jeffrey R. Reimers

Biquinoxalinylyl bridged bis-porphyrins are weakly coupled systems as is required for incorporation of this porphyrin-linkage in chemical PRC models.





2788 2794

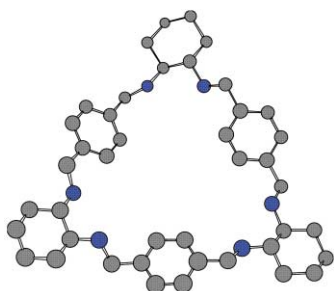


Syntheses and solid state structures of cyclic diynes with two chalcogen centres – a competition between weak interactions

J. Hilko Schulte, Daniel B. Werz, Frank Rominger and Rolf Gleiter

A competition between weak interactions in the solid state structure of cyclic diynes with two chalcogen centres is reported.

2795 2800

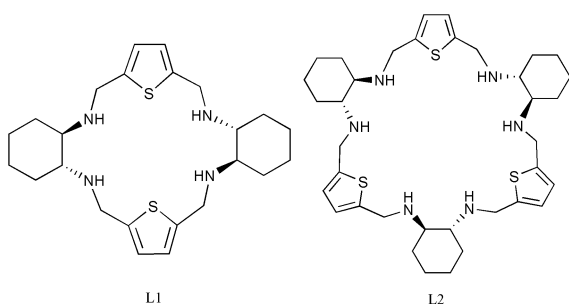


Self-assembly of achiral and chiral macrocyclic ligands: synthesis, protonation constants, conformation and asymmetric catalysis

Jian Gao and Arthur E. Martell

A new type of achiral and chiral polyaza macrocyclic ligands was synthesized, and the chiral ligand shown to be an effective auxiliary for a direct asymmetric catalytic aldol reaction.

2801 2806



Novel chiral N₄S₂- and N₆S₃-donor macrocyclic ligands: synthesis, protonation constants, metal-ion binding and asymmetric catalysis in the Henry reaction

Jian Gao and Arthur E. Martell

New hydrophobic chiral macrocyclic ligands **L1–L3** have been synthesized by the Schiff base condensation approach.

2807

Emma Vickerstaffe, Brian H. Warrington,
Mark Ladlow and Steven V. Ley

Fully automated multi-step solution phase synthesis using polymer supported reagents: preparation of histone deacetylase inhibitors

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