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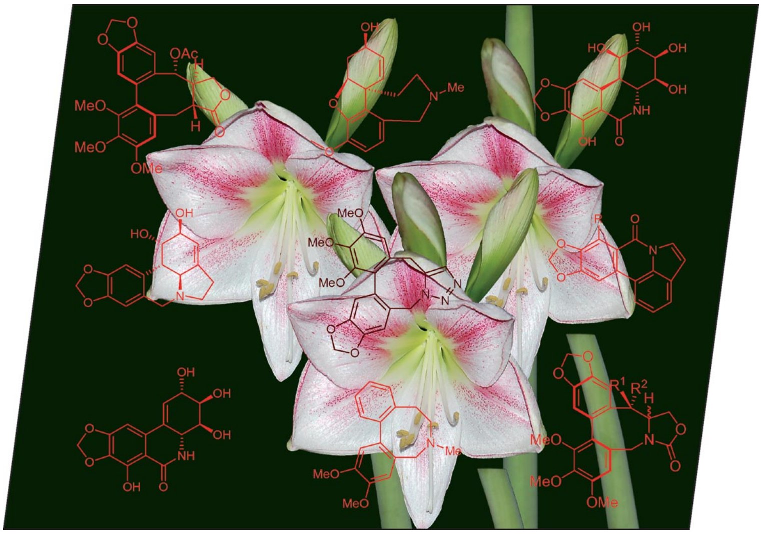
A union formed by chemical societies in Europe (ChemPubSoc Europe) has taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry*. Three further members of ChemPubSoc Europe (Austria, Czech Republic and Sweden) are Associates of the two journals.

COVER PICTURE

The cover picture shows flowers belonging to the *crinum* family, a member of the well-known *amaryllidaceae* family, in the background. A number of naturally occurring alkaloids with very intriguing biological potential have been isolated from the amaryllidaceae family of flowers. The structures shown in the foreground of the cover picture are some representative examples of amaryllidaceae alkaloids, such as narciclassine, hippadine, lycorine etc., as well as a few unnatural analogues bearing close structural similarity to some of the amaryllidaceae alkaloids. Details of some of the structures and the recent advances in the synthesis of some of the unnatural and yet structurally similar alkaloid analogues are presented in the Microreview by P. Appukkuttan and E. Van der Eycken on p. 5867ff.



CONTENTS

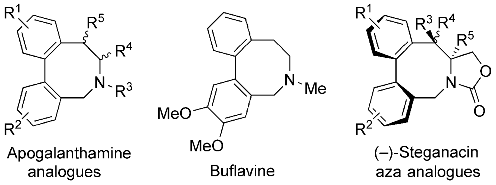
MICROREVIEW

Natural Products

P. Appukkuttan,
E. Van der Eycken* 5867–5886

An Overview of Syntheses of Apogalanthamine Analogues and 7-Aza Derivatives of Steganacin and Steganone

Keywords: Alkaloids / Natural products / Amaryllidaceae / Apogalanthamine / Buflavine / Steganone



A critical overview of the developments in the synthesis of apogalanthamine analogues and steganacin and steganone 7-aza analogues over the last four decades is presented. These amaryllidaceae alkaloid analogues bear a 5,6,7,8-tetrahydrodibenzo[*c*,*e*]azocine skeleton and are well known for their diverse and potent biological activities.

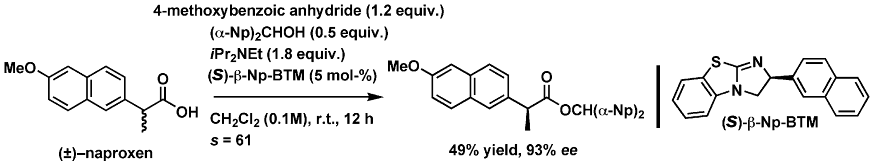
SHORT COMMUNICATION

Chiral NSAIDs

I. Shiina,* K. Nakata,
Y. Onda 5887–5890

Kinetic Resolution of Racemic Carboxylic Acids Using Achiral Alcohols by the Promotion of Benzoic Anhydrides and Tetramisole Derivatives: Production of Chiral Nonsteroidal Anti-Inflammatory Drugs and Their Esters

Keywords: Kinetic resolution / Carboxylic acids / Anhydrides



An environmentally friendly protocol was developed to directly provide chiral carboxylic esters from racemic free carboxylic acids and achiral alcohols by utilizing a transacylation process to generate mixed anhydrides from acid components and benzoic anhydride derivatives in the presence of organocatalysts without the use of harmful metallic promoters.

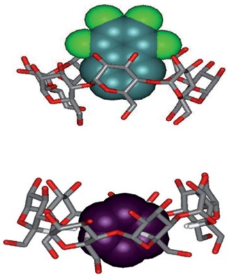
FULL PAPERS

Aromatic Inclusion Compounds

J. P. Ribeiro, S. Bacchi, G. Dell'Anna,
M. Morando, F. J. Cañada, F. Cozzi,*
J. Jiménez-Barbero* 5891–5898

A Combined NMR, Computational, and HPLC Study of the Inclusion of Aromatic and Fluoroaromatic Compounds in Cyclodextrins as a Model for Studying Carbohydrate–Aromatic Interactions

Keywords: Cyclodextrins / Inclusion compounds / Host-guest systems / Molecular modelling / Molecular dynamics



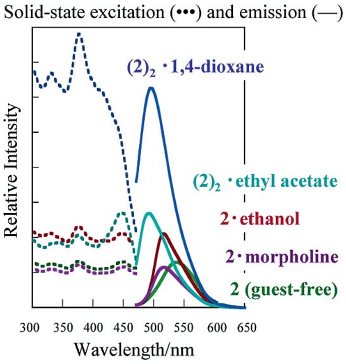
Cyclodextrins provide an excellent model to study sugar···aromatic interactions. Dispersion forces between the aromatic ring and the sugar C–H bonds strongly influence recognition ability with a major destabilization of the complex taking place when the aromatic ring holds fluorine atoms.

Fluorescent Clathrate Hosts

Y. Ooyama,* S. Nagano, M. Okamura, K. Yoshida* 5899–5906

Solid-State Fluorescence Changes of 2-(4-Cyanophenyl)-5-[4-(diethylamino)phenyl]-3*H*-imidazo[4,5-*a*]naphthalene upon Inclusion of Organic Solvent Molecules

Novel imidazo[4,5-*a*]naphthalene-type fluorescent clathrate host **2**, with two possible tautomeric forms (**A** and **B**) of the imidazole ring, exhibits sensitive colour change and drastic fluorescence enhancement behaviour with a blueshift in the emission maximum upon enclathration of various kinds of organic solvent molecules.



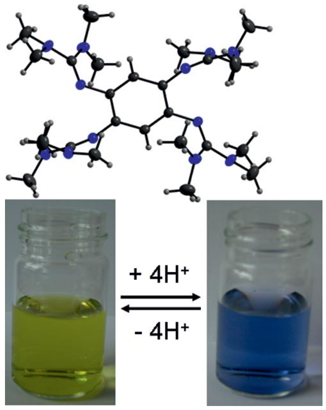
Keywords: Dyes / Clathrates / Nitrogen heterocycles / Fluorescence / Inclusion compounds

Molecular Electron Donors

A. Peters, E. Kaifer, H.-J. Himmel* 5907–5914

1,2,4,5-Tetrakis(tetramethylguanidino)benzene: Synthesis and Properties of a New Molecular Electron Donor

The molecular electron donor 1,2,4,5-tetrakis(tetramethylguanidino)benzene changes its colour upon protonation; it is green in the diprotonated form and blue in the tetraprotonated form and can be readily oxidised.



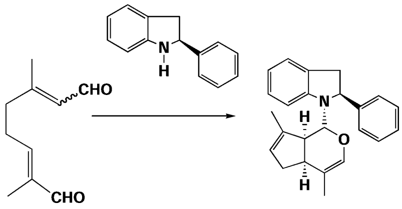
Keywords: Organic electron donors / Guanidines / Oxidation / Protonation

Iridoid Synthesis

E. M. Santangelo, I. Liblikas, A. Mudalige, K. W. Törnroos, P.-O. Norrby, C. R. Unelius* 5915–5921

Asymmetric Synthesis of Iridoid Derivatives Using Resolved 2-Phenylindoline as a Chiral Auxiliary

An asymmetric synthetic route to iridoids has been developed. It includes the resolution of 2-phenylindoline that hitherto has not been used as a chiral inductor and an intramolecular cycloaddition that gives three enantiopure stereocenters in one step.



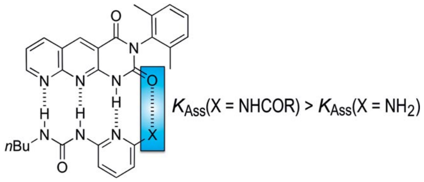
Keywords: Iridoid / Cycloaddition reaction / Nepetalactol / Chromatographic resolution / 2-Phenylindoline

Molecular Recognition

J. Taubitz, U. Lüning* 5922–5927

On the Importance of the Nature of Hydrogen Bond Donors in Multiple Hydrogen Bond Systems

Association constants for the reaction between a fourfold hydrogen bond receptor possessing an AADA hydrogen bond pattern and several complementary partners have been determined by NMR titration and by isothermal titration calorimetry (ITC).



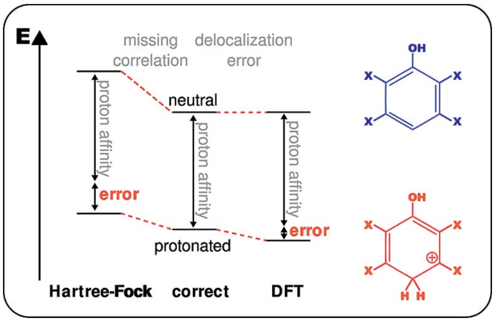
Keywords: Association constant / Hydrogen bond / Isothermal titration calorimetry (ITC) / NMR titration / Supramolecular chemistry

Prediction of Substituent Effects

T. Schwabe, S. Grimme* 5928–5935

Theoretical Description of Substituent Effects in Electrophilic Aromatic Substitution Reactions

Keywords: Phenol / Proton affinity / Electrophilic substitution / Ab initio and DFT calculations / Double-hybrid density functionals



Appropriate quantum chemical models are needed to predict very accurate proton affinities of multiply substituted phenols and also to reach chemical accuracy for relative values or regioselectivities. The description of delocalization and −I/+I effects requires an accurate account of electron-correlation effects.

PEGylated Peptides

J. Krüger,* T. Minuth, W. Schröder, J. Werwath 5936–5945

Manufacturing and PEGylation of a Dual-Acting Peptide for Diabetes

Keywords: Peptides / Solid-phase synthesis / Synthesis design / Mixed-phase synthesis / Fragment synthesis

H-His-Ser-Gln-Gly-Thr-Phe-Thr-Ser-Asp-Tyr-Ala-Arg-Tyr-Leu-Asp-Ala-Arg-
Arg-Ala-Arg-Glu-Phe-Ile-Lys-Trp-Leu-Val-Arg-Gly-Arg-Cys-(PEG$_{43KD}$)-OH

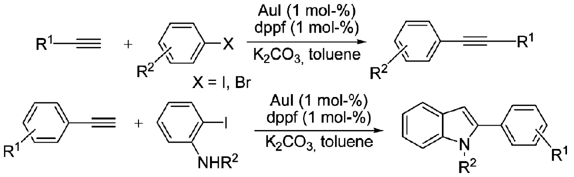
Production of complex peptides at scale within a reasonable economic framework is still a challenge. We present the development of a mixed-phase synthesis for a PEGylated 31mer peptide. The process has a wide scope and is applicable for large scale synthesis.

Gold-Catalyzed C−C Coupling

P. Li, L. Wang,* M. Wang, F. You 5946–5951

Gold(I) Iodide Catalyzed Sonogashira Reactions

Keywords: C−C coupling / Gold / Alkynes / Nitrogen heterocycles



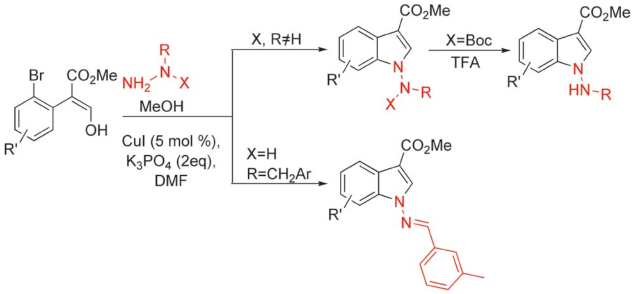
Gold(I) iodide catalyzed Sonogashira reactions of terminal alkynes with aryl iodides and bromides have been described. The reactions proceeded smoothly in the presence of AuI and dppf in toluene and generated the corresponding cross-coupling products in excellent yields. Aromatic terminal alkynes also reacted with 2-iodoaniline to form indoles after cyclization.

Indole Synthesis

F. Melkonyan, A. Topolyan, M. Yurovskaya, A. Karchava* 5952–5956

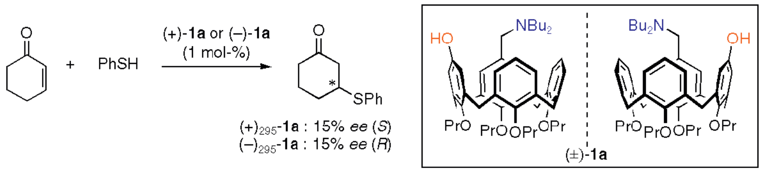
Synthesis of 1-Amino-1*H*-indole-3-carboxylates by Copper(I)-Catalyzed Intramolecular Amination of Aryl Bromides

Keywords: C−N coupling / Copper / Nitrogen heterocycles / Annulation / Indoles



Simple access to various *N*-substituted 1-amino-1*H*-indole-3-carboxylates was established by use of copper(I)-catalyzed intramolecular *N*-arylation. For the preparation of *N*-mono-substituted and *N*-unsubstituted derivatives, the cyclization of Boc-protected enehydrazines and subsequent deprotection were applied.

Inherently Chiral Calixarenes



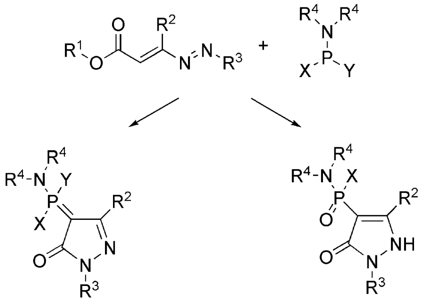
Newly designed, inherently chiral calix[4]arenes have been synthesized and resolved to optically pure forms. The enantiomeric recognition ability of one chiral calix[4]arene was examined with mandelic acid by ^{1}H NMR spectroscopy. In addition, the chiral calix[4]arenes were used in asymmetric reactions as organocatalysts.

S. Shirakawa, A. Moriyama,
S. Shimizu* 5957–5964

Synthesis, Optical Resolution and Enantiomeric Recognition Ability of Novel, Inherently Chiral Calix[4]arenes: Trial Application to Asymmetric Reactions as Organocatalysts

Keywords: Calixarenes / Chiral resolution / Host–guest systems / Asymmetric catalysis / Michael addition / Organocatalysis

Phosphorylated Pyrazolones



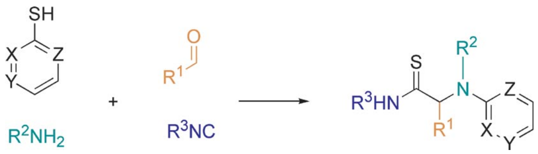
On account of the biological importance of organophosphorus heterocycles, we describe herein a practical access to 5-oxo-4-phoshoranylidene-4,5-dihydro-1*H*-pyrazoles and (3-oxo-2,3-dihydro-1*H*-pyrazol-4-yl)phosphonamidates through the reaction of 1,2-diaza-1,3-butadienes with aminophosphorus nucleophiles.

O. A. Attanasi,* G. Baccolini, C. Boga,
L. De Crescentini,* G. Giorgi,
F. Mantellini, S. Nicolini 5965–5973

Reaction of 1,2-Diaza-1,3-butadienes with Aminophosphorus Nucleophiles: A Practical Access to New Phosphorylated Pyrazolones

Keywords: Diazabutadienes / Phosphorus / Ylides / Michael addition / Hydrazones / Pyrazolones

Ugi–Smiles Coupling



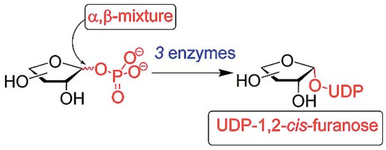
The use of the Smiles rearrangement in Ugi-type couplings with aromatic mercaptans allows for the straightforward, multicomponent formation of α-arylamino thiocarboxamides. The scope of this new four-component coupling is further broadened with the use of heterocyclic mercapto derivatives that afford thioamides of high biological interest in one step.

A. Barthelon, L. El Kaïm,* M. Gizolme,
L. Grimaud* 5974–5987

Thiols in Ugi- and Passerini–Smiles-Type Couplings

Keywords: Ugi reaction / Smiles reaction / Isocyanides / Rearrangement / Thiols / Multicomponent reactions

Rare Glycoconjugates



The first stereoselective chemoenzymatic syntheses of UDP-α-D-galactofuranose, UDP-β-L-arabinofuranose, UDP-α-D-fucofuranose and UDP-α-D-6F-galactofuranose, starting from anomeric mixtures of the corresponding furanosyl 1-phosphates, are described.

P. Peltier, J.-P. Guégan,
R. Daniellou,* C. Nugier-Chauvin,*
V. Ferrières 5988–5994

Stereoselective Chemoenzymatic Synthesis of UDP-1,2-*cis*-furanoses from α,β-Furanosyl 1-Phosphates

Keywords: Carbohydrates / Nucleotides / Glycoconjugates / Enzyme catalysis

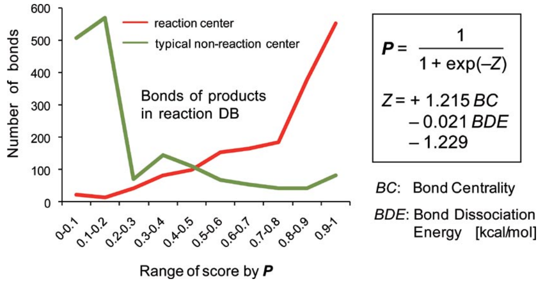
CONTENTS

Synthesis Design

A. Tanaka,* T. Kawai, T. Matsumoto, M. Fujii, T. Takabatake, H. Okamoto, K. Funatsu* 5995–6007

Construction of a Statistical Evaluation Model Based on Molecular Centrality to Find Retrosynthetically Important Bonds in Organic Compounds

Keywords: Synthesis design / Molecular centrality / Bond centrality / Bond dissociation energy / Retrosynthesis / Molecular complexity



$$P = \frac{1}{1 + \exp(-Z)}$$

$$Z = +1.215\,BC - 0.021\,BDE - 1.229$$

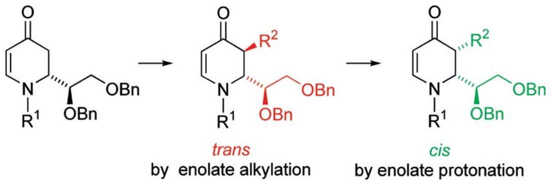
The evaluation equation to determine retrosynthetically important bonds has been constructed from reaction databases by logistic regression analysis. The equation consists of bond centrality and bond dissociation energy terms.

Asymmetric Synthesis

P. Etayo, R. Badorrey, M. D. Díaz-de-Villegas,* J. A. Gálvez* 6008–6014

Stereoselective Synthesis of Chiral 2,3-Disubstituted 2,3-Dihydro-4(1*H*)-pyridones

Keywords: Asymmetric synthesis / Enolate alkylation / Piperidines / Stereoselectivity / Synthetic methods



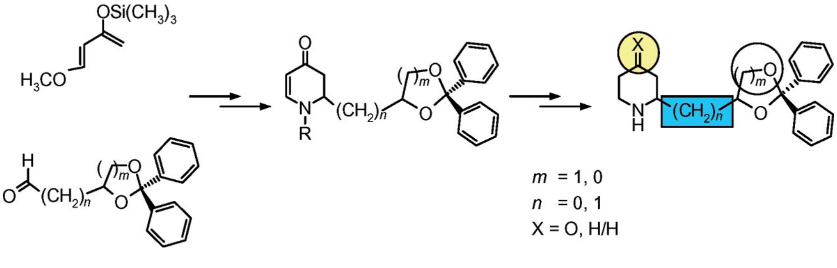
The asymmetric synthesis of 2,3-disubstituted 2,3-dihydropyridones of *trans* and *cis* configuration in enantiomerically pure form is reported.

Dexoxadrol Derivatives

M. Sax, R. Fröhlich, D. Schepmann, B. Wünsch* 6015–6028

💻 Synthesis and NMDA Receptor Affinity of Ring and Side Chain Homologues of -Dexoxadrol

Keywords: Receptors / Hetero-Diels–Alder reaction / Danishefsky's diene / Structure–affinity relationships / Oxygen heterocycles



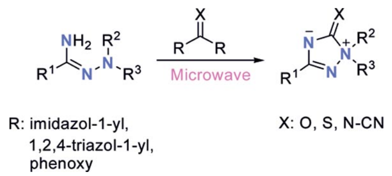
Dexoxadrol derivatives with an expanded oxygen heterocycle (1,3-dioxane instead of 1,3-dioxolane), an enlarged distance between the two heterocycles, and an additional oxo group in the 4-position of the piperidine ring were synthesized and pharmacologically evaluated. These derivatives showed considerable loss of affinity towards the phencyclidine binding site of an NMDA receptor.

Triazolium Ylides

M. Khankischpur, T. Kurz* 6029–6033

Convenient Microwave-Assisted Synthesis of 5-Functionalized 1,2,4-Triazolium -Ylides Starting from *N′*,*N′*-Disubstituted Carbohydrazonamides

Keywords: Ylides / Nitrogen heterocycles / Cyclization / Microwave-assisted synthesis



5-Functionalized 1,2,4-triazolium ylides can be prepared in good yields and very short reaction times from *N′*,*N′*-disubstituted carbohydrazonamides and 1,1′-carbonylbis(1,2,4-triazole), 1,1′-thiocarbonyldiimidazole or diphenyl *N*-cyanimidocarbonate under microwave irradiation.

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* Author to whom correspondence should be addressed.

💻 Supporting information on the WWW (see article for access details).