

# Organic & Biomolecular Chemistry

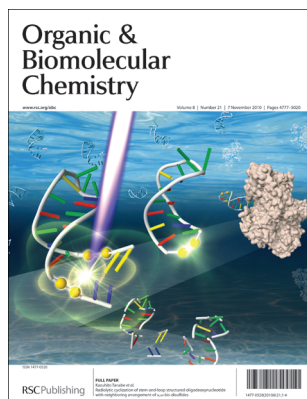
An international journal of synthetic, physical and biomolecular organic chemistry

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## IN THIS ISSUE

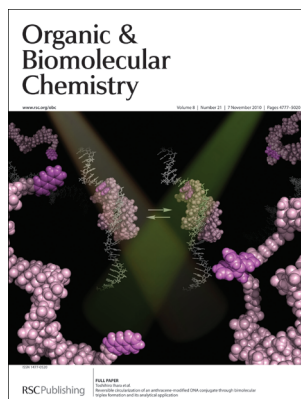
ISSN 1477-0520 CODEN OBCRAK 8(21) 4777–5020 (2010)



### Cover

See Kazuhito Tanabe *et al.*, pp. 4837–4842.  
X-Ray irradiation of an aqueous solution of modified oligodeoxynucleotides with a pair of disulfides at both ends causes efficient cyclization via an intramolecular exchange reaction.

Image reproduced by permission of Kazuhito Tanabe from *Org. Biomol. Chem.*, 2010, **8**, 4837.



### Inside cover

See Toshihiro Ihara *et al.*, pp. 4843–4848.  
The oligonucleotide conjugate was reversibly circularized through photodimerization of the anthracenes attached on both ends. This process would be potentially useful as a probe reaction with high specificity and sensitivity.

Image reproduced by permission of Toshihiro Ihara from *Org. Biomol. Chem.*, 2010, **8**, 4843.

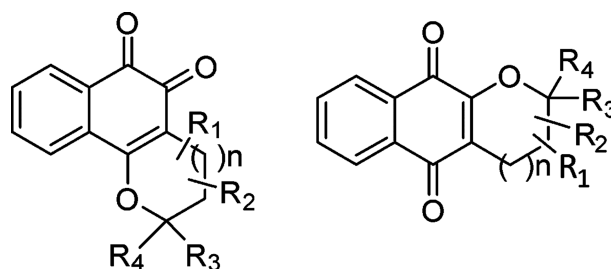
## PERSPECTIVE

4793

### Strategies for the synthesis of bioactive pyran naphthoquinones

Vitor Francisco Ferreira,\* Sabrina Baptista Ferreira and Fernando de Carvalho da Silva

Strategies for the synthesis of bioactive pyran naphthoquinones.



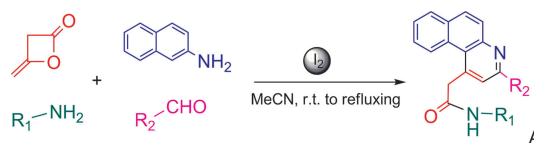
## COMMUNICATIONS

4803

### A domino synthesis of benzoquinolinamide in the presence of iodine

Li-Yan Zeng and Chun Cai\*

Iodine catalyzed domino reaction of diketene, amine, aromatic aldehyde and naphthalenamine for the synthesis of benzoquinolinamides in one-pot.



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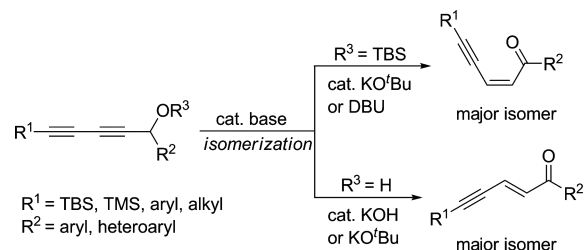
## COMMUNICATIONS

4806

**Stereoselective synthesis of enynones *via* base-catalyzed isomerization of 1,5-disubstituted-2,4-pentadiynyl silyl ethers or their alcohol derivatives**

Jingjin Chen, Guoqin Fan and Yuanhong Liu\*

Base-catalyzed stereoselective synthesis of enynones from 1,5-disubstituted-2,4-pentadiynyl silyl ethers or their alcohol derivatives has been developed.

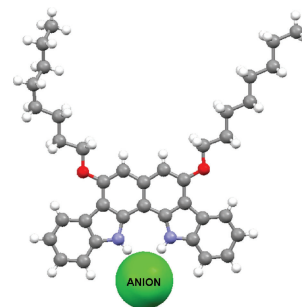


4811

**A new building block for anion supramolecular chemistry. Study of carbazolocarbazole as anion receptor**

David Curiel,\* Miriam Más-Montoya, Guzmán Sánchez, Raúl A. Orenes, Pedro Molina and Alberto Tárraga

Carbazolo[1,2-*a*]carbazole has been evaluated as an anion receptor in DMF. Anion binding studies have been contrasted by several experimental techniques.

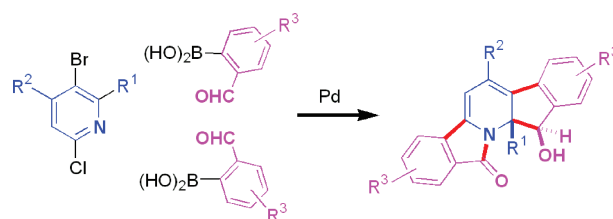


4815

**Synthesis of new pentacyclic chromophores through a highly regio- and diastereoselective cascade process**

Zein el abidine Chamas, Olivier Dietz, Emmanuel Aubert, Yves Fort and Victor Mamane\*

Four bonds and two stereocenters with *trans* relationship are produced during a cascade process leading to pentacyclic chromophores.

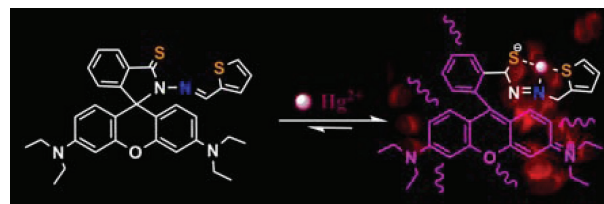


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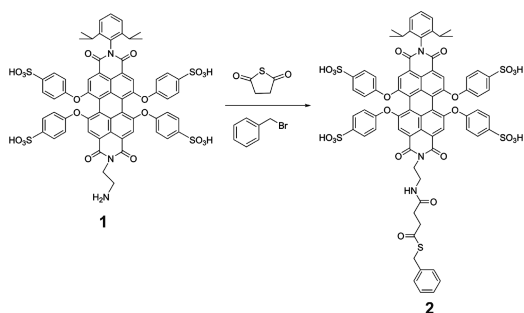
**A thiophen-thioxorhodamine conjugate fluorescent probe for detecting mercury in aqueous media and living cells**

Yi Zhou, Xue-Yan You, Yuan Fang, Ju-Ying Li, Ke Liu and Cheng Yao\*

A ratiometric fluorescent Hg<sup>2+</sup> sensor **RB-S2** which featured the high affinity of Hg<sup>2+</sup> to sulfur-containing rhodamine and dual-responsive in both aqueous media and living cells was developed.



4823

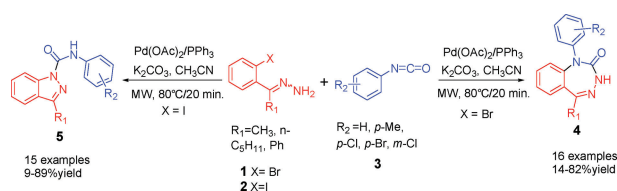


### Site-specific incorporation of perylene into an N-terminally modified light-harvesting complex II

Kalina Peneva, Kristina Gundlach, Andreas Herrmann, Harald Paulsen and Klaus Müllen\*

Employing the utility of the native chemical ligation, site-specific attachment of an ultrastable perylene dye to a derivative of the major light-harvesting complex (LHCII) was demonstrated.

4827

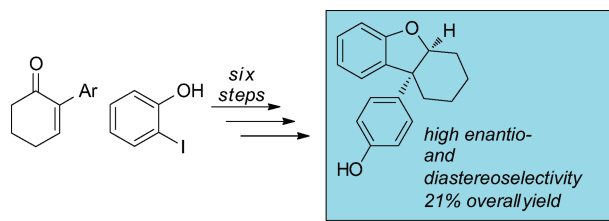


### Facile synthesis of 1,3,4-benzotriazepines and 1-arylamide-1H-indazoles via palladium-catalyzed cyclization of aryl isocyanates and aryl hydrazones under microwave irradiation

Chune Dong,\* Lingli Xie, Xiaohong Mou, Yashan Zhong and Wei Su

A strategy involving palladium-catalyzed cyclization of halophenyl hydrazones and aryl isocyanates provides convenient synthesis of 1,3,4-benzotriazepines (4) or 1-arylamide-1H-indazoles (5) in one step under microwave irradiation.

4831

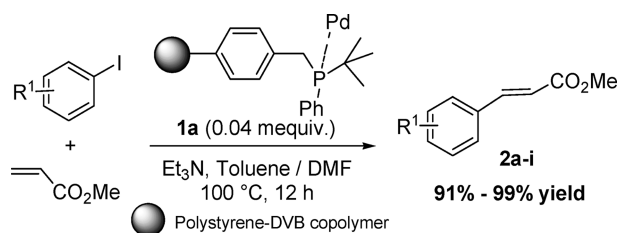


### Asymmetric synthesis of a tricyclic benzofuran motif: a privileged core structure in biologically active molecules

Henrik Sundén and Roger Olsson\*

An efficient synthetic strategy for the asymmetric synthesis of a hexahydrodibenzofuran core structure, with a quaternary stereogenic center.

4834



### Reusable polystyrene-supported Pd catalyst for Mizoroki-Heck reactions with extremely low amounts of supported Pd

Carine Diebold, Stéphane Schweizer, Jean-Michel Becht\* and Claude Le Drian\*

Heck reactions of aryl iodides using extremely low amounts of supported Pd (0.04 mequiv.) are reported. The catalyst can be reused successfully up to three times.

# Prizes and Awards

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The Organic Chemistry awards portfolio rewards excellence in both industry and academia, for original research in any aspect of organic chemistry as well as specific areas including organometallic and physical organic chemistry.

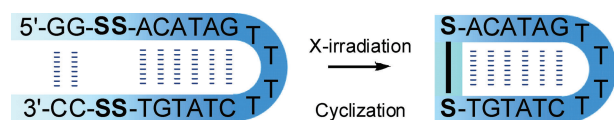
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4837

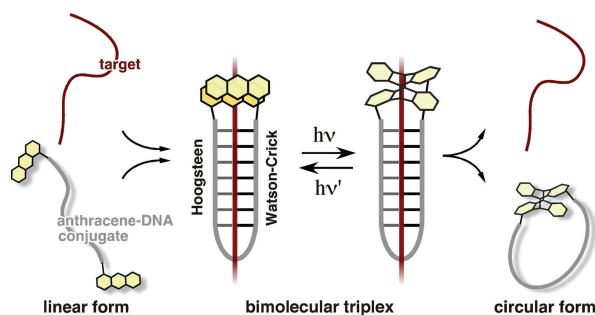


### Radiolytic cyclization of stem-and-loop structured oligodeoxynucleotide with neighboring arrangement of $\alpha,\omega$ -bis-disulfides

Kazuhiro Tanabe,\* Eiji Matsumoto, Takeo Ito and Sei-ichi Nishimoto\*

Modified oligodeoxynucleotides bearing a pair of disulfides that form a stem-and-loop structure underwent efficient cyclization upon X-ray irradiation.

4843

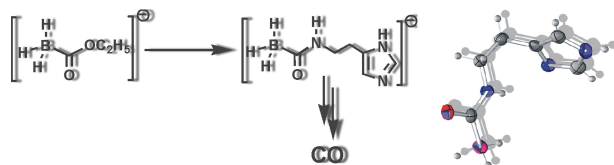


### Reversible circularization of an anthracene-modified DNA conjugate through bimolecular triplex formation and its analytical application

Pelin Arslan, Akinori Jyo and Toshihiro Ihara\*

The conformation of anthracene–DNA conjugate was topologically locked as the circular form by photoreaction. The sequence selectivity of the reaction was higher than that of the duplex system with similar thermal stability.

4849

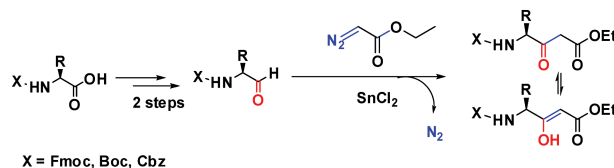


### Syntheses, structural characterization and CO releasing properties of boranocarbonate $[H_3BCO_2H]^-$ derivatives

Tamil Selvi Pitchumony, Bernhard Spingler, Roberto Motterlini and Roger Alberto\*

Boranocarbamates, derivatives of boranocarbonate  $[H_3BCO_2H]^-$  release CO in water at a slower rate than the parent, opening thereby new opportunities for biological applications.

4855



### Tin(II) chloride assisted synthesis of N-protected $\gamma$ -amino $\beta$ -keto esters through semipinacol rearrangement

Anupam Bandyopadhyay, Neha Agrawal, Sachitanand M. Mali, Sandip V. Jadhav and Hosahudya N. Gopi\*

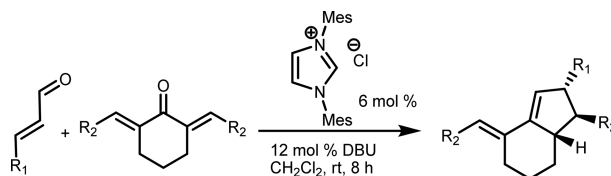
Facile and efficient synthesis of N-protected  $\gamma$ -amino  $\beta$ -keto esters through semipinacol rearrangement

4861

### NHC-catalysed annulation of enals to tethered dienones: efficient synthesis of bicyclic dienes

Vijay Nair,\* Sreekumar Vellalath, Beneesh P. Babu, Vimal Varghese, Rony Rajan Paul and Eringathodi Suresh

Homoenolates generated from  $\alpha,\beta$ -unsaturated aldehydes using NHC catalysis underwent facile addition to dibenzylidene cyclohexanone to afford bicyclic cyclopentenes as single diastereomers.

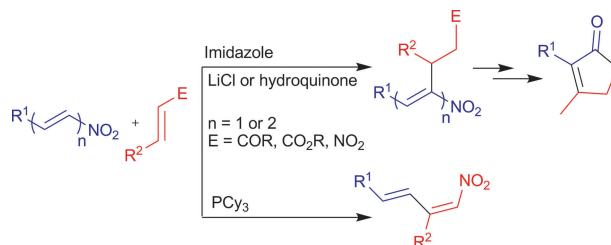


4867

### Rauhut–Currier type homo- and heterocouplings involving nitroalkenes and nitrodienes

Pramod Shanbhag, Pradeep R. Nareddy, Mamta Dadwal, Shaikh M. Mobin and Irishi N. N. Namboothiri\*

Amine and phosphine mediated dimerization of nitroalkenes and amine mediated coupling of nitroalkenes with other activated alkenes under mild conditions lead to synthetically useful products.

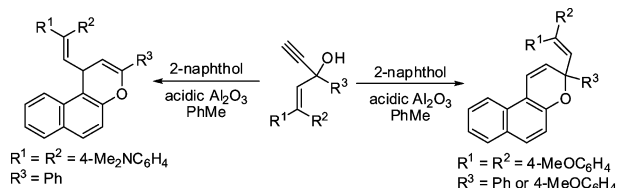


4874

### The influence of a 1,1-diarylvinyloxy moiety on the photochromism of naphthopyrans

Christopher D. Gabbutt, B. Mark Heron,\* Colin Kilner and Suresh B. Kolla

Photochromic (1,1-diarylvinyloxy) substituted naphthopyrans have been prepared from the condensation of triaryl enynols with naphthols.  $\lambda_{\text{max}}$  of the derived photomerocyanines is bathochromically shifted.

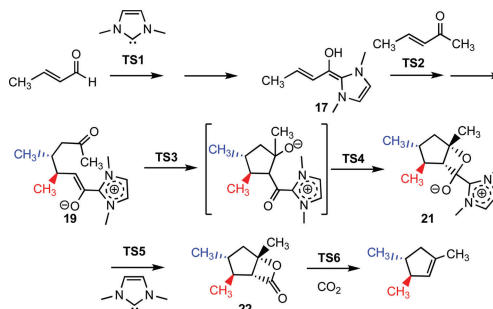


4884

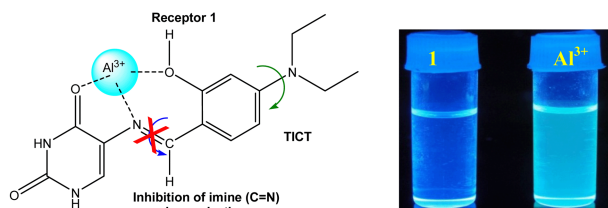
### Understanding the mechanism of stereoselective synthesis of cyclopentenes *via* N-heterocyclic carbene catalyzed reactions of enals with enones

Luis R. Domingo,\* Ramón J. Zaragoza and Manuel Arnó

The nucleophilic attack of the Breslow intermediate **17** to enones is responsible for the *trans* stereoselectivity experimentally observed.



4892

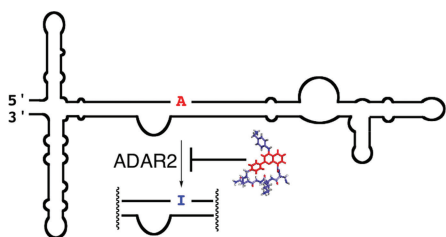


### Pyrimidine based highly sensitive fluorescent receptor for $\text{Al}^{3+}$ showing dual signalling mechanism

K. K. Upadhyay\* and Ajit Kumar

A pyrimidine based fluorescent probe (receptor 1) detected  $\text{Al}^{3+}$  selectively in DMSO as well as in aqueous media with its lowest detection limit of the order of  $10^{-10}$  M and  $10^{-9}$  M respectively. Receptor 1 is the first ever example where a single molecular probe is able to show imine ( $\text{C}=\text{N}$ ) isomerization inhibition along with twisted intramolecular charge transfer (TICT) in combinatorial fashion.

4898

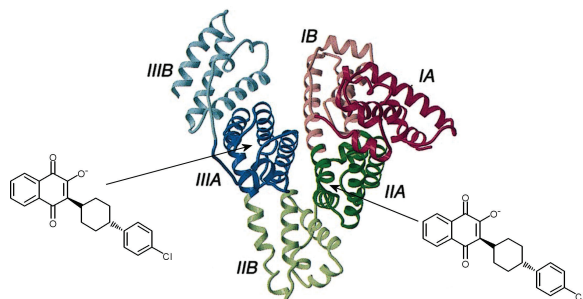


### Selective inhibition of ADAR2-catalyzed editing of the serotonin 2c receptor pre-mRNA by a helix-threading peptide

Nicole T. Schirle, Rena A. Goodman, Malathy Krishnamurthy and Peter A. Beal\*

A first example of substrate-selective inhibition of editing by an RNA-binding small molecule, which sets the stage for the development of new reagents capable of controlling gene function through manipulation of mRNA editing

4905

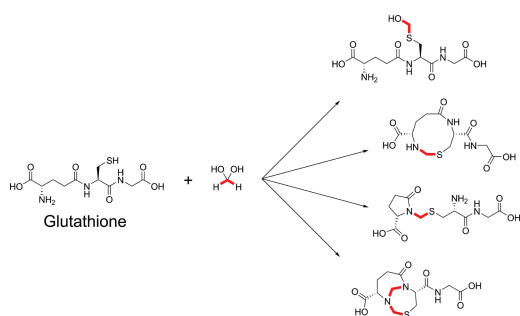


### Combination of chiroptical, absorption and fluorescence spectroscopic methods reveals multiple, hydrophobicity-driven human serum albumin binding of the antimalarial atovaquone and related hydroxynaphthoquinone compounds

Ferenc Zsila\* and Ilona Fitos

Induced circular dichroism spectra indicated the serum albumin binding of two atovaquone molecules with equally high affinity.

4915



### Studies on the reaction of glutathione and formaldehyde using NMR

Richard J. Hopkinson, Philippa S. Barlow, Christopher J. Schofield\* and Timothy D. W. Claridge\*

The reaction of glutathione and formaldehyde is shown to produce a number of products, including two new cyclic adducts.



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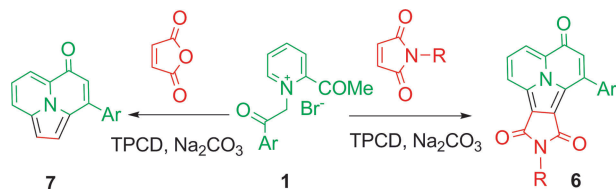
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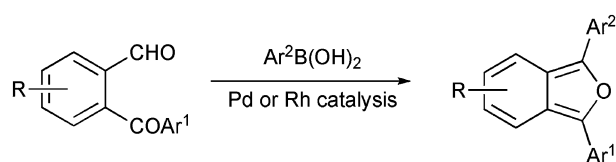


### Synthesis of 1,2-annulated and 1,2-unsubstituted pyrrolo[2,1,5-*de*]quinolizin-5-ones (cycl[3.3.2]azin-5-ones) via [3+2] cycloadditions of 1-oxoquinolizinium ylides with cyclic alkenes

Yun Liu, Hua-You Hu, Yan Zhang, Hong-Wen Hu and Jian-Hua Xu\*

1,2-Annulated and 1,2-unsubstituted pyrrolo[2,1,5-*de*]quinolizin-5-ones have been synthesized by one pot tandem reactions of 2-acetyl-*N*-phenacylpyridinium bromides with electron-deficient cyclic alkenes.

4927



### Regiospecific synthesis of functionalised 1,3-diarylbenzofurans via palladium- and rhodium-catalysed reaction of boronic acids with *o*-acylbenzaldehydes under thermal or microwave activation

Jérôme Jacq, Bernard Bessières, Cathy Einhorn and Jacques Einhorn\*

Variously substituted 1,3-diarylbenzofurans have been regiospecifically prepared via palladium- and rhodium-catalysed reaction of functionalised boronic acids onto *o*-acylbenzaldehydes, using classical or microwave heating.

4934

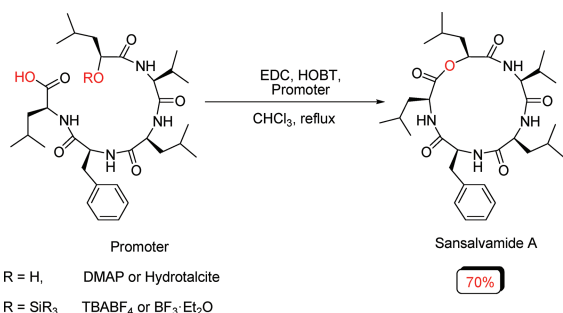


### Radical formation of amino acid precursors in interstellar regions? Ser, Cys and Asp

Daniel J. Knowles, Tianfang Wang and John H. Bowie\*

Theoretical calculations indicate that favourable reactions between  $\text{NH}_2\cdot\text{CHCN}$  and  $\text{R}\cdot$  ( $\text{R} = \text{CH}_2\text{OH}$ ,  $\text{CH}_2\text{SH}$  and  $\text{CH}_2\text{CN}$ ) should produce the Ser, Cys and Asp precursors  $\text{NH}_2\text{CH}(\text{R})\text{CN}$

4940



### Highly efficient macrolactonization of $\omega$ -hydroxy acids using benzotriazole esters: synthesis of Sansalvamide A

José Antonio Morales-Serna, Ericka Sánchez, Ricardo Velázquez, Jorge Bernal, Eréndira García-Ríos, Rubén Gaviño, Guillermo Negrón-Silva and Jorge Cárdenas\*

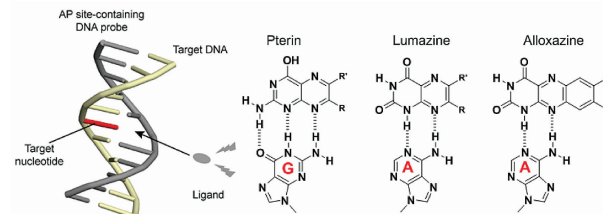
A facile and mild macrolactonization reaction of  $\omega$ -hydroxy acids in the presence of EDC/HOBT was developed. The reactions were performed under basic, neutral and acidic conditions.

4949

### Effect of substituents of alloxazine derivatives on the selectivity and affinity for adenine in AP-site-containing DNA duplexes

Burki Rajendar, Arivazhagan Rajendran, Zhiqiang Ye, Eriko Kanai, Yusuke Sato, Seichi Nishizawa, Marek Sikorski and Norio Teramae\*

Alloxazine can bind to adenine selectively, whereas its methylated ligand, lumichrome, selectively binds to thymine over A, C and G opposite an AP site in DNA duplexes. Such changes in the base-selectivity and binding affinities are discussed.

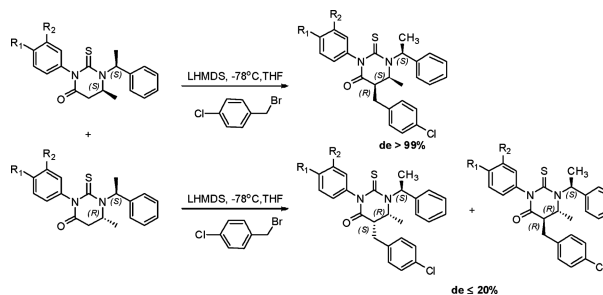


4960

### Diastereoselective syntheses of 3-aryl-5-(aryllalkyl)-6-methyl-1-(1-phenylethyl)-thioxotetrahydropyrimidin-4(1H)-ones: A stereochemical perspective from *endo* and *exocyclic* chiral centres

Varun Kumar, Pallegogu Raghavaiah, Shaikh M. Mobin and Vipin A. Nair\*

The orientations of the exocyclic and endocyclic groups dictate the stereochemical outcome of the reaction.

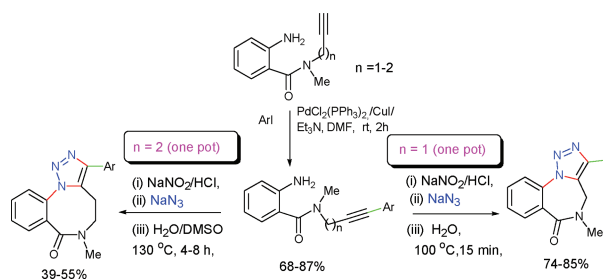


4971

### An expedient and facile route for the general synthesis of 3-aryl substituted 1,2,3-triazolo[1,5-*a*][1,4]benzodiazepin-6-ones and 1,2,3-triazolo[1,5-*a*][1,5]benzodiazocin-7-ones

Chinmay Chowdhury,\* Anup Kumar Sasmal and Basudeb Achari

An efficient route for the general synthesis of 3-aryl substituted 1,2,3-triazolo[1,5-*a*][1,4]benzodiazepin-6-ones and 1,2,3-triazolo[1,5-*a*][1,5]benzodiazocin-7-ones was developed.

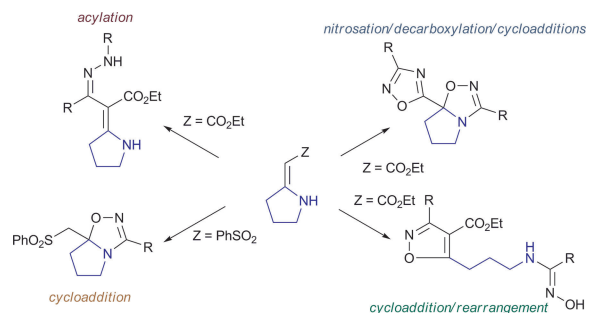


4978

### Reaction of heterocyclic enamines with nitrile oxide and nitrilimine precursors

Cevher Altuğ, Yasar Dürüst, Mark C. Elliott,\* Benson M. Kariuki, Tillique Rorstad and Mark Zaal

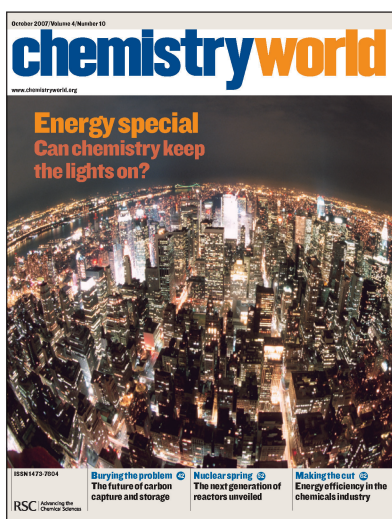
Alkylidenepyrrrolidines react with nitrile oxide and nitrilimine precursors to give a range of heterocyclic products.



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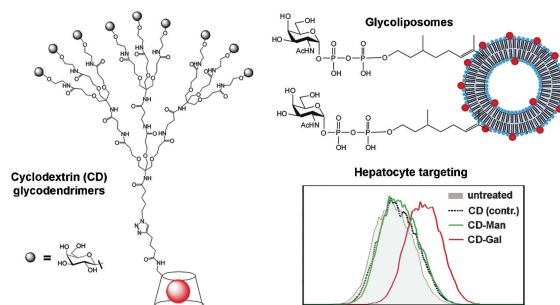
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4987

### Design, synthesis and biological evaluation of carbohydrate-functionalized cyclodextrins and liposomes for hepatocyte-specific targeting

Gonçalo J. L. Bernardes, Raghavendra Kikkeri, Maha Magliano, Paola Laurino, Mayeul Collot, Sung You Hong, Bernd Lepenies and Peter H. Seeberger\*

Targeting glycan-binding receptors is an attractive strategy for cell-specific drug and gene delivery. In this study, we designed, synthesised and evaluated novel carbohydrate-functionalized  $\beta$ CDs and liposomes for hepatocyte-specific delivery.

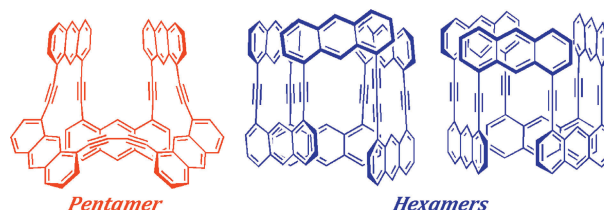


4997

### Chemistry of anthracene–acetylene oligomers. XVII. Synthesis, structure, and dynamic behavior of 1,8-anthrylene pentamers and hexamers with acetylene linkers

Shinji Toyota,\* Takahiro Kawakami, Risa Shinnishi, Rie Sugiki, Shinya Suzuki and Tetsuo Iwanaga

Anthrylene pentamers and hexamers with acetylene linkers were synthesized by cyclization with coupling reactions. The structure and the dynamic behavior of the macrocyclic oligomers were investigated.

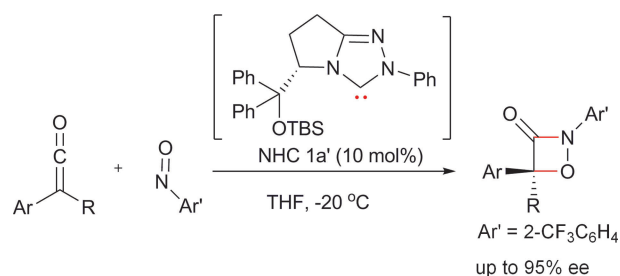


5007

### Enantioselective formal [2+2] cycloaddition of ketenes with nitroso compounds catalyzed by N-heterocyclic carbenes

Tong Wang, Xue-Liang Huang and Song Ye\*

Chiral N-heterocyclic carbenes were found to be efficient catalysts for the formal [2+2] cycloaddition reaction of alkyl(aryl)ketenes and nitroso compounds to give the corresponding 1,2-oxazetidin-3-ones in moderate to good yields with high enantioselectivities.

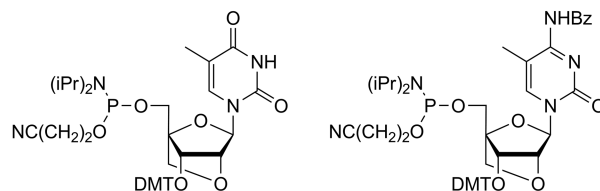


5012

### LNA 5'-phosphoramidites for 5'→3'-oligonucleotide synthesis

Andreas Stahl Madsen,\* T. Santhosh Kumar and Jesper Wengel

Efficient synthesis of LNA thymine and LNA 5-methylcytosine 5'-phosphoramidites, allowing incorporation into oligonucleotides synthesized in the 5'→3' direction. Key steps include regioselective enzymatic benzylation of the 5'-hydroxy group of unprotected LNA thymine, and subsequent quantitative 4,4'-dimethoxytritylation of the 3'-hydroxy group of the O5'-benzoylated LNA thymine nucleoside.



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