

IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (20) 2521–2636 (2005)



Cover

See Fabrizio Mancin, Paolo Scrimin, Paolo Tecilla and Umberto Tonellato, page 2540.

Chemists have taken up the fascinating challenge to develop artificial metallonucleases capable of competing with the natural enzymes. The picture shows a dicerium complex cleaving a DNA double strand. Image reproduced by permission of Paolo Tecilla *et al.*, from *Chem. Commun.*, 2005, 2540.



Inside cover

See Rohan T. Ranasinghe, David A. Rusling, Vicki E. C. Powers, Keith R. Fox and Tom Brown, page 2555. Pyrrolopyrimidine nucleoside analogues are synthesised and show selective CG base pair recognition in DNA triplexes. Image reproduced by permission of Tom Brown *et al.*, from *Chem. Commun.*, 2005, 2555.

EDITORIAL

2539

New journal *Molecular BioSystems* has arrived

ChemComm is pleased to announce that the first issue of its sister journal *Molecular BioSystems* is now published.



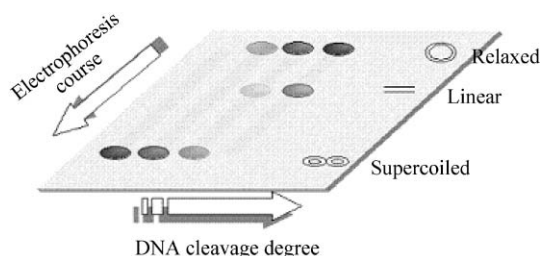
FEATURE ARTICLE

2540

Artificial metallonucleases

Fabrizio Mancin, Paolo Scrimin, Paolo Tecilla and Umberto Tonellato

Since the first report on the ability of metal ions to promote DNA hydrolysis, tremendous progress toward obtaining efficient synthetic DNA hydrolytic agents has been attained. However, several aspects need to be addressed before artificial catalysts are able to challenge the natural enzymes. This *Feature Article* highlights the progress toward the realization of synthetic nucleases with particular attention to the strategies that can be pursued to improve efficiency and selectivity.



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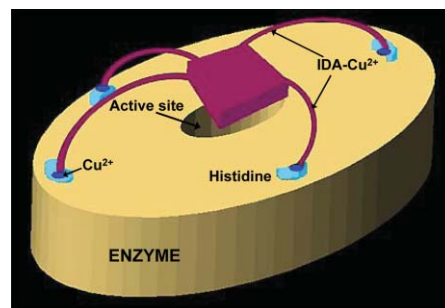
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Inhibition of matrix metalloproteinase-9 by “multi-prong” surface binding groups

Abir L. Banerjee, Shakila Tobwala, Manas K. Haldar, Michael Swanson, Bidhan C. Roy, Sanku Mallik* and D. K. Srivastava*

A novel approach for blocking the active site accessibility of MMP-9 (but not MMP-10) and inhibiting the enzyme by “multi-prong” IDA-Cu²⁺ containing ligands is demonstrated.

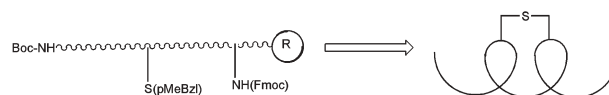


2552

Synthesis of constrained helical peptides by thioether ligation: application to analogs of gp41

Florence M. Brunel and Philip E. Dawson*

We present a procedure to constrain peptides in a helical conformation using thioether ligation. This simple, high-yielding method represents an attractive alternative to the use of lactam constraints.

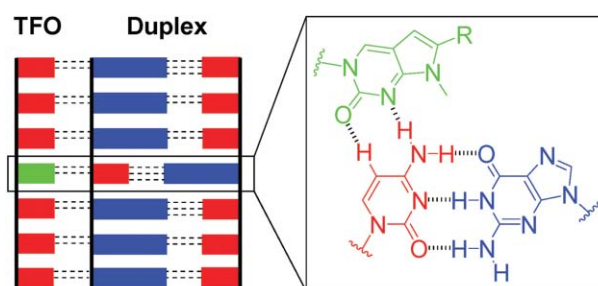


2555

Recognition of CG inversions in DNA triple helices by methylated 3*H*-pyrrolo[2,3-*d*]pyrimidin-2(7*H*)-one nucleoside analogues

Rohan T. Ranasinghe, David A. Rusling, Vicki E. C. Powers, Keith R. Fox and Tom Brown*

Substituted 3*H*-pyrrolo[2,3-*d*]pyrimidin-2(7*H*)-one nucleoside analogues have been synthesised from 5-alkynyl-uridine derivatives, incorporated into triplex forming oligonucleotides (TFOs) and found to selectively bind CG inversions with enhanced affinity compared to T.

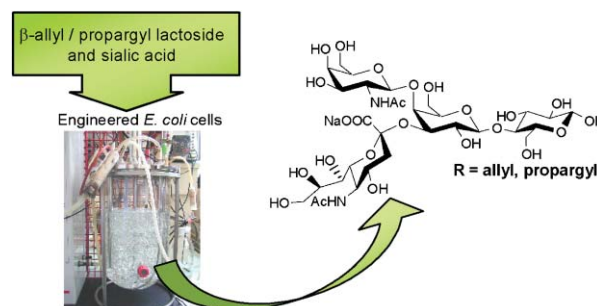


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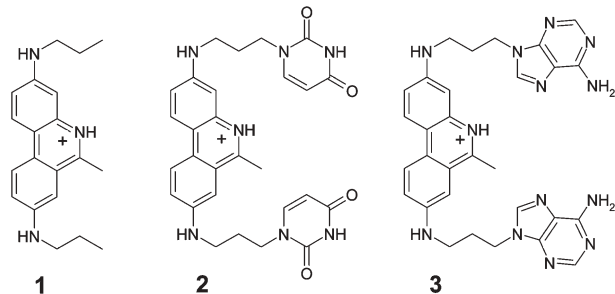
Biosynthesis of conjugatable saccharidic moieties of GM₂ and GM₃ gangliosides by engineered *E. coli*

Sébastien Fort,* LEMONIA Birikaki, Marie-Pierre Dubois, Tatiana Antoine, Eric Samain and Hugues Driguez

Oligosaccharidic portions of gangliosides GM₂ and GM₃ bearing allyl or propargyl aglycons, are biosynthesized on the gram scale by growing metabolically engineered *Escherichia coli* cells.



2561

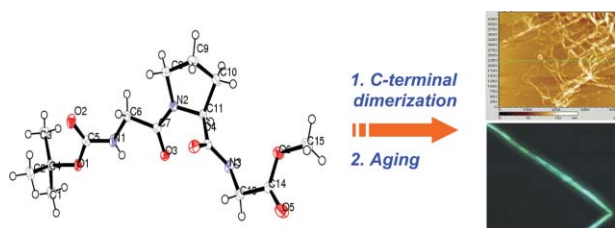


Recognition of homo-polynucleotides containing adenine by a phenanthridinium bis-uracil conjugate in aqueous media

Lidija-Marija Tumir, Ivo Piantanida,* Iva Juranović, Zlatko Meić, Sanja Tomić and Mladen Žinić*

A bis-uracil–phenanthridinium conjugate **2** significantly more strongly stabilized ds-polynucleotides containing poly-dA and poly-AH⁺ strands than adenine analogue **3** and reference **1**, consecutive adenines in polynucleotide being essential for the observed selectivity.

2564

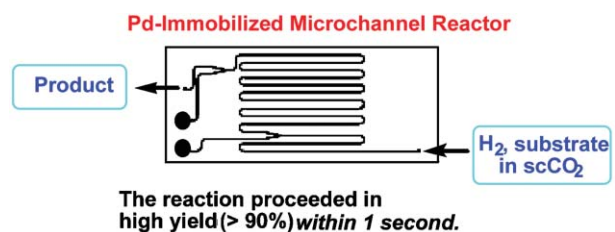


Enforcing solution phase nanoscopic aggregation in a palindromic tripeptide

K. Krishna Prasad, C. S. Purohit, Alok Jain, R. Sankaramakrishnan and Sandeep Verma*

This report describes nanosized fibril formation by a tripeptide conjugate derived from the highly evolutionary conserved V3 loop of HIV-1.

2567

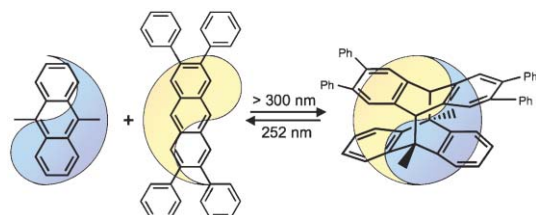


Hydrogenation reactions using scCO₂ as a solvent in microchannel reactors

Juta Kobayashi, Yuichiro Mori and Shū Kobayashi*

We developed an effective microfluidic hydrogenation system using scCO₂ as a reaction medium. It is remarkable that the reaction took place very rapidly (mean residence time: less than 1 second).

2569



Complementarity in bimolecular photochromism

David Bailey and Vance E. Williams*

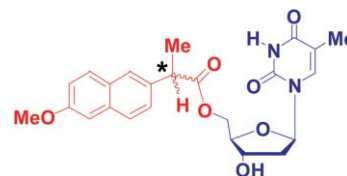
Irradiating 2,3,6,7-tetraphenylanthracene in the presence of 9,10-dimethylantracene leads to exclusive formation of the cross-dimer. No photochemical reaction is observed when either of these chromophores is irradiated in the absence of the other.

2572

Stereo-differentiation in the excited state behaviour of naphthalene-thymine dyads

Susana Encinas, Maria J. Climent, Noureddine Belmadoui and Miguel A. Miranda*

Chiral discrimination has been found in the photophysical processes involving the naphthalene excited states of the title dyads: singlet deactivation by hydrogen bonding molecules, singlet energy transfer and triplet decay.

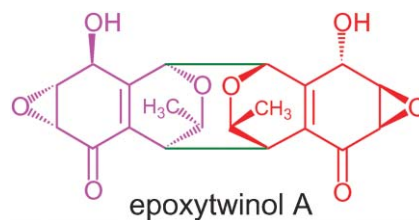


2575

Epoxytwinol A, a novel unique angiogenesis inhibitor with C_2 symmetry, produced by a fungus

Hideaki Kakeya,* Rie Onose, Hiroyuki Koshino and Hiroyuki Osada*

We isolated a novel unique pentaketide dimer designated as epoxytwinol A from the fermentation broth of a fungus. Its structure was determined to have a new carbon skeleton with C_2 symmetry *via* spectroscopic evidence. Epoxytwinol A inhibited endothelial cell migration stimulated by vascular endothelial growth factor ($ED_{100} = 2.6 \mu\text{M}$).

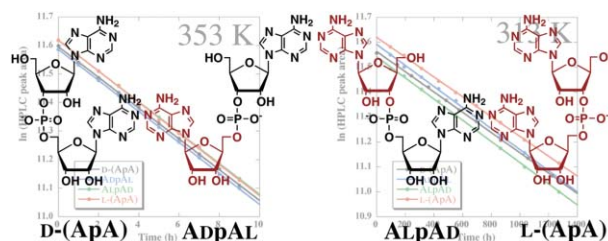


2578

Kinetic analysis of hydrolytic reaction of homo- and heterochiral adenylyl(3'-5')adenosine isomers: breaking homochirality reduces hydrolytic stability of RNA

Hidehito Urata,* Rie Sasaki, Hiroyo Morita, Marina Kusumoto, Yoko Ogawa, Kozue Mitsuda and Masao Akagi*

The hydrolytic stabilities of the diastereomeric isomers of adenylyl(3'-5')adenosine were carefully compared and the preferential hydrolysis of the heterochiral dimers over the homochiral ones was observed.

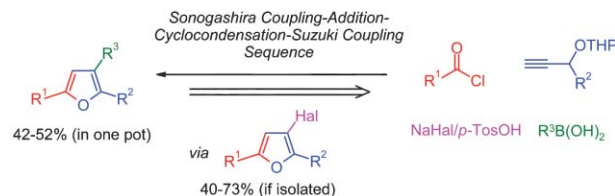


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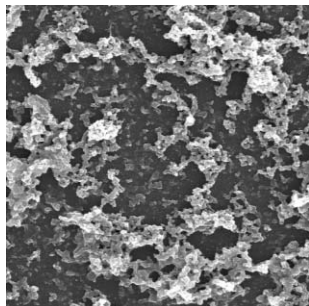
A novel one-pot three-component synthesis of 3-halofurans and sequential Suzuki coupling

Alexei S. Karpov, Eugen Merkul, Thomas Oeser and Thomas J. J. Müller*

A novel Sonogashira–electrophilic addition sequence to ynones with concomitant deprotection and cyclocondensation opens a new one-pot synthesis of 3-halofurans and a sequential one-pot Sonogashira–addition–cyclocondensation–Suzuki reaction to furnish 2,3,5-trisubstituted furans.



2584

**Direct electrochemistry and electrocatalysis with hemoglobin in water-soluble quantum dots film on glassy carbon electrode**

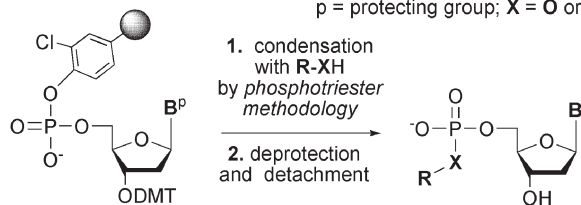
Qing Lu, Shengshui Hu,* Daiwen Pang and Zhike He

The direct electrochemistry of hemoglobin can be performed by immobilizing hemoglobin in a water-soluble quantum dots (CdSe–ZnS) film on glassy carbon electrode.

2586



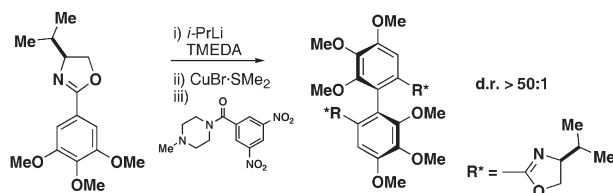
p = protecting group; X = O or NH

**An efficient solid phase synthesis of 5'-phosphodiester and phosphoramidate monoester nucleoside analogues**

Lorenzo De Napoli, Giovanni Di Fabio,* Jennifer D'Onofrio and Daniela Montesarchio

An easy and efficient strategy to obtain libraries of 5'-phosphodiester and 5'-phosphoramidate monoester nucleoside analogues in a highly pure form has been developed, starting from a new nucleoside based solid support.

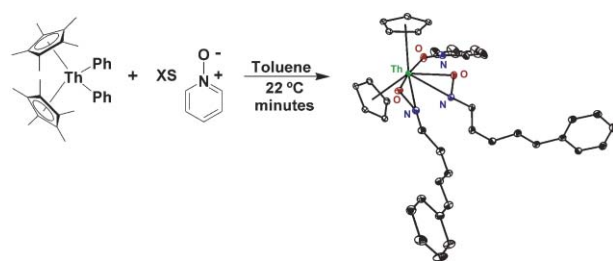
2589

**Aryl–aryl coupling via directed lithiation and oxidation**

David S. Surry, David J. Fox, Simon J. F. Macdonald and David R. Spring*

Organocuprates formed by a directed lithiation–transmetalation sequence may be oxidised to give biaryls. Inter- and intramolecular reactions are both successful and a highly diastereoselective reaction is possible if a valinol-derived chiral oxazoline is used as a directing group.

2591

**Carbon–nitrogen bond cleavage in pyridine ring systems mediated by organometallic thorium(IV) complexes**

Jaime A. Pool, Brian L. Scott and Jaqueline L. Kiplinger*

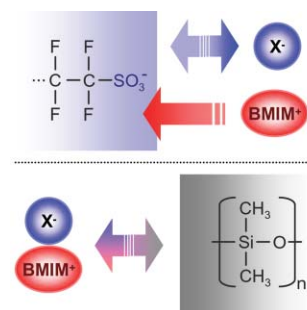
Thorium(IV) alkyl and aryl complexes of the type (C₅Me₅)₂ThR₂ (R = CH₂Ph, Ph) have been found to mediate the facile ring-opening and dearomatization of the pyridine ring of pyridine *N*-oxide under ambient conditions to afford the first thorium η²-(*O,N*)-oximate complexes.

2594

Elucidating interactions of ionic liquids with polymer films using confocal Raman spectroscopy

Thomas Schäfer,* Roberto E. Di Paolo, Ricardo Franco and João G. Crespo

Ionic liquids and membranes are materials for emerging cleaner processing and composites in sensors, but little is known about their molecular interaction. Using confocal Raman microscopy, it was revealed how ionic liquids interact with PDMS and Nafion[®] membranes.

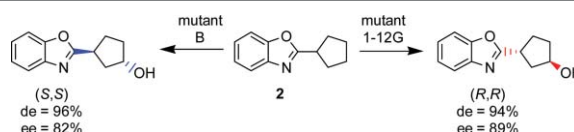


2597

Stereoselective hydroxylation of an achiral cyclopentanecarboxylic acid derivative using engineered P450s BM-3

Dieter F. Münzer, Peter Meinhold, Matthew W. Peters, Sabine Feichtenhofer, Herfried Griengl, Frances H. Arnold,* Anton Glieder and Anna de Raadt*

Substrate engineered, achiral carboxylic acid derivative **2** was biohydroxylated with various mutants of cytochrome P450 BM-3 to give two out of the four possible diastereoisomers in high de and ee.

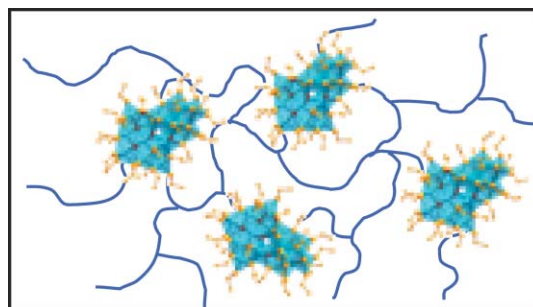


2600

New hybrid organic–inorganic nanocomposites based on functional [Ti₁₆O₁₆(OEt)₂₄(OEMA)₈] nano-fillers

Sergio Bocchini, Giulia Fornasieri, Laurence Rozes, Sondes Trabelsi, Jocelyne Galy, Nick E. Zafeiropoulos, Manfred Stamm, Jean-François Gérard and Clément Sanchez*

New hybrid nanocomposites based on a methacrylate functionalized titanium-oxo cluster as nano-cross-linker show improved mechanical properties, optical transparency and photochromic activity.

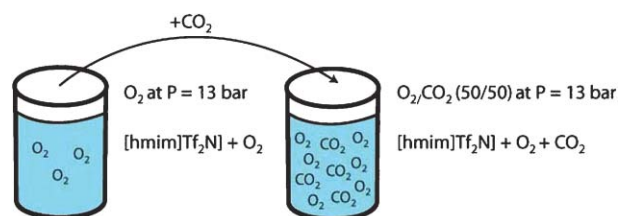


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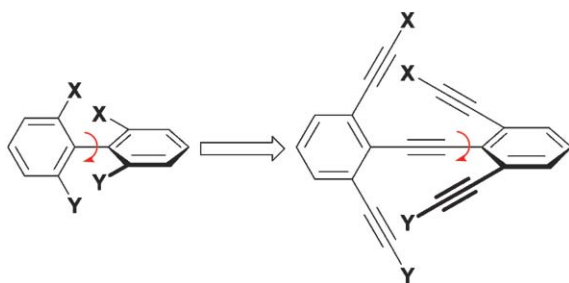
Enhancement of oxygen and methane solubility in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide using carbon dioxide

Daniel G. Hert, Jessica L. Anderson, Sudhir N. V. K. Aki and Joan F. Brennecke*

Low pressure CO₂ can be used to increase the solubility of gases like O₂ and CH₄ in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide.



2606

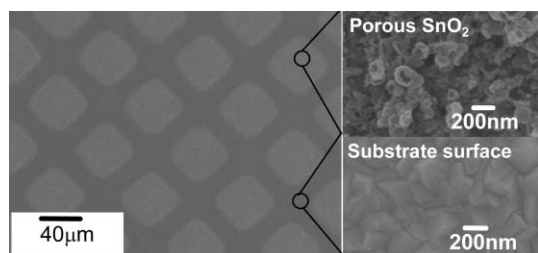


Hindered rotation in an “exploded” biphenyl

Ognjen Š. Miljanić, Sangdon Han, Daniel Holmes, Gaston R. Schaller and K. Peter C. Vollhardt*

The first cases of hindered rotation around the triple bond in simple diphenylacetylenes were observed, including that in chiral 2,2'-bis(trimethylsilyl)-6,6'-bis(dimethylhexylsilyl)diphenylacetylene.

2609

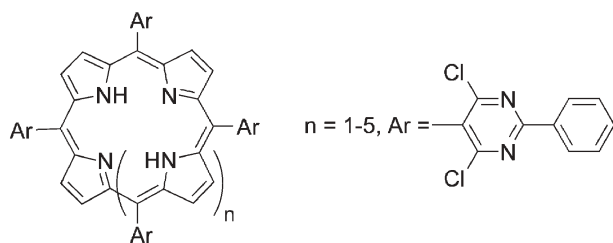


Fabrication of highly porous and micropatterned SnO₂ films by oxygen bubbles generated on the anode electrode

Eiji Hosono, Shinobu Fujihara, Hiroaki Imai, Itaru Honma and Haoshen Zhou*

Porous SnO₂ films and patterned films are fabricated by electrochemical assisted chemical bath deposition.

2612

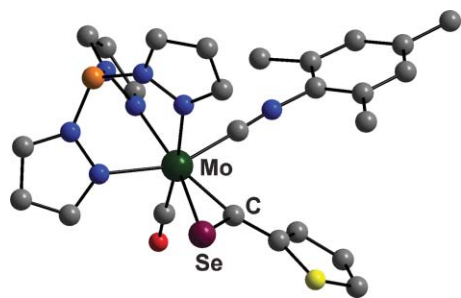


meso-Dichloropyrimidinyl substituted expanded porphyrins

Wouter Maes, Jeroen Vanderhaeghen and Wim Dehaen*

4,6-Dichloro-2-phenylpyrimidine-5-carbaldehyde can be used for the synthesis of novel *meso*-aryl substituted expanded porphyrins and the introduction of this heteroaromatic moiety shows great potential for the simplification and extension of post-macrocyclization synthetic modifications.

2615



Selenoaryl complexes of molybdenum

Lorraine M. Caldwell, Anthony F. Hill* and Anthony C. Willis

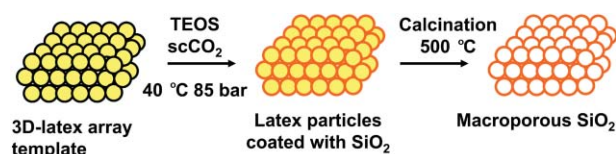
The reaction of mesityl isoselenocyanate with molybdenum alkylidynes provides the first structurally characterised examples of mononuclear selenoaryl complexes, which may also be obtained directly from elemental selenium in the presence of a catalytic amount of mesityl isocyanide.

2618

Synthesis of ordered macroporous SiO₂ in supercritical CO₂ using 3D-latex array templates

Albertina Cabañas,* Eduardo Enciso, M. Carmen Carbajo, M. José Torralvo, Concepción Pando and Juan Antonio R. Renuncio

Ordered macroporous SiO₂ membranes have been produced for the first time by the decomposition of silicon alkoxides in supercritical carbon dioxide (scCO₂) using 3D-latex array templates.

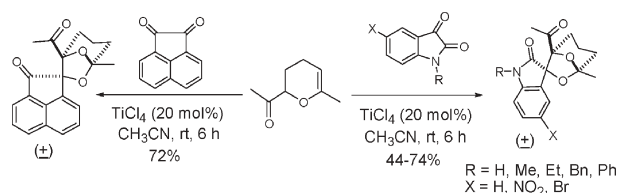


2621

TiCl₄ catalyzed tandem construction of C–C and C–O bonds: a simple and one-pot atom-economical stereoselective synthesis of spiro-oxindoles

Deevi Basavaiah,* Jamjanam Srivardhana Rao, Raju Jannapu Reddy and Anumolu Jaganmohan Rao

An atom-economical stereoselective synthesis of [1-acetyl-5-methyl-6,8-dioxabicyclo(3.2.1)octane]-7-spiro-3'-(indolin-2'-one)] derivatives, containing both the oxindole and 6,8-dioxabicyclo(3.2.1)octane moieties *via* TiCl₄ catalyzed coupling of 2-acetyl-6-methyl-2,3-dihydro-4*H*-pyran with isatin derivatives, involving tandem construction of C–C and C–O bonds, is described.



2624

The rhodium catalyzed three-component reaction of diazoacetates, titanium(IV) alkoxides and aldehydes

Chong-Dao Lu, Hui Liu, Zhi-Yong Chen, Wen-Hao Hu* and Ai-Qiao Mi

The Rh(II)-catalyzed three-component reaction of diazoacetates, titanium alkoxides and aldehydes is shown to give α -alkoxyl- β -hydroxyl acid derivatives. The novel C–C bond formation reaction is proposed to occur through oxonium ylides derived from diazo compounds and titanium alkoxides, followed by intermolecular trapping by aldehydes.

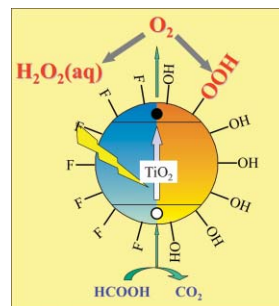


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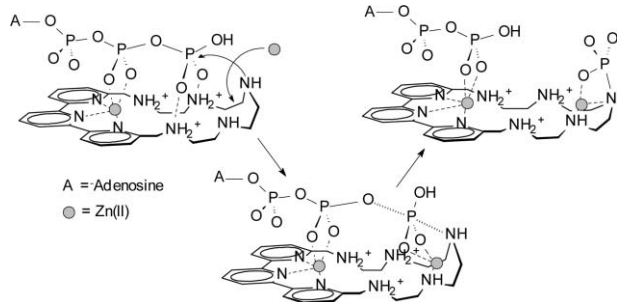
Sustained production of H₂O₂ on irradiated TiO₂ – fluoride systems

Valter Maurino,* Claudio Minero, Giuseppe Mariella and Ezio Pelizzetti

The UV irradiation of fluorinated anatase TiO₂ in water, in the presence of O₂ and a hole scavenger, leads to the photocatalytic production of H₂O₂ with steady state concentration levels up to 1.3 × 10^{−3} M. Without fluoride the H₂O₂ formation is not detectable. Fluoride ion inhibits H₂O₂ surface complexation and hinders ≡Ti–OOH formation, a key species for H₂O₂ degradation.



2630

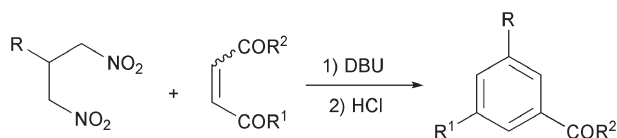


A zinc(II)-based receptor for ATP binding and hydrolysis

Carla Bazzicalupi, Andrea Bencini,* Antonio Bianchi,* Andrea Danesi, Claudia Giorgi, Carlos Lodeiro, Fernando Pina, Samuele Santarelli and Barbara Valtancoli

A protonated Zn(II) complex with a terpyridine-containing macrocycle catalyses ATP hydrolysis only in the presence of a second Zn(II) ion, which acts as cofactor assisting the phosphoryl transfer from ATP to an amine group of the macrocycle.

2633



One pot synthesis of 3,5-alkylated acetophenone and methyl benzoate derivatives *via* an anionic domino process

Roberto Ballini,* Luciano Barboni,* Dennis Fiorini, Guido Giarlo and Alessandro Palmieri

The one pot synthesis of 3,5-alkylated acetophenones and methyl benzoate derivatives starting from 1,3-dinitroalkanes and 2-ene-1,4-dicarbonyl derivatives is reported. The reactions occur *via* an anionic domino process.

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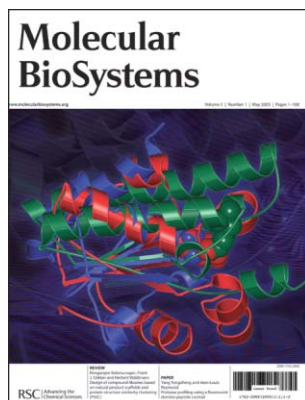
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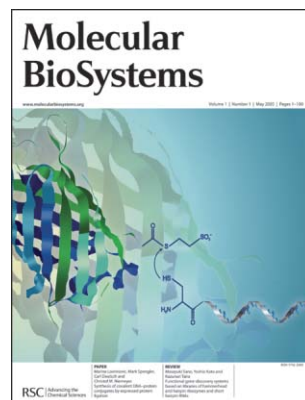
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**Cover**

See Herbert Waldmann *et al.*, page 36. Clustering of protein domain cores according to structural similarity (here Cdc25A (red), 11 β HSD1 (green), and AChE (blue)) is a new guiding principle for guiding compound library development for chemical biology and medicinal chemistry. Image reproduced by permission of Rengarajan Balamurugan, Frank J. Dekker and Herbert Waldmann, from *Mol. BioSyst.*, 2005, 1, 36.

**Inside cover**

See Christof M. Niemeyer *et al.*, page 64. The synthesis of covalent DNA-protein conjugates is accomplished by expressed protein ligation of intein-fusion proteins and a DNA-cysteine conjugate. Image reproduced by permission of Marina Lovrinovic, Mark Spengler, Carl Deutsch and Christof M. Niemeyer, from *Mol. BioSyst.*, 2005, 1, 64.

EDITORIAL

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Chemistry meets the -omic sciences and systems biology

Welcome to the first issue of *Molecular BioSystems*—an exciting new chemical biology journal with a particular focus on the interface between chemistry and the -omic sciences and systems biology.



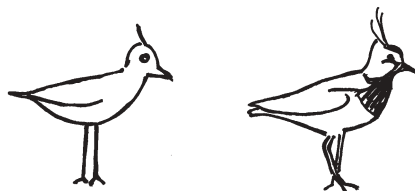
HOT OFF THE PRESS

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Hot off the Press

In the *Hot off the Press* section of *Molecular BioSystems*, members of the Editorial Board and their research groups highlight recent literature for the benefit of the community. This month the highlighted topics include enhancing the efficacy of RNA interference, identification of targets of kinase inhibitors, analysis of low-abundance peptides, and secretion of recombinant proteins.

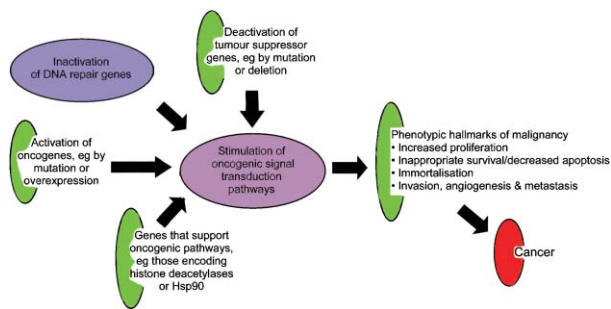
HOT
OFF THE PRESS



Feedback dynamics and cell function: Why systems biology is called Systems Biology

Olaf Wolkenhauer* and Mihajlo Mesarović

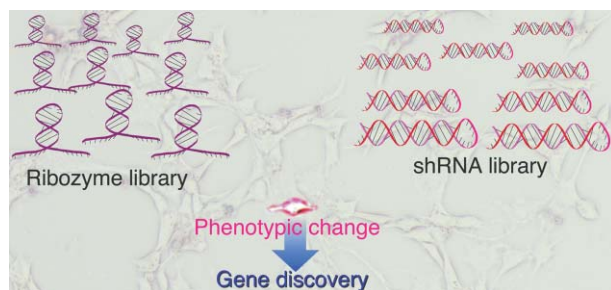
Systems Biology is not the application of engineering principles to biology, but a merger of systems- and control theory with molecular- and cell biology.



Genomics and the second golden era of cancer drug development

Paul Workman

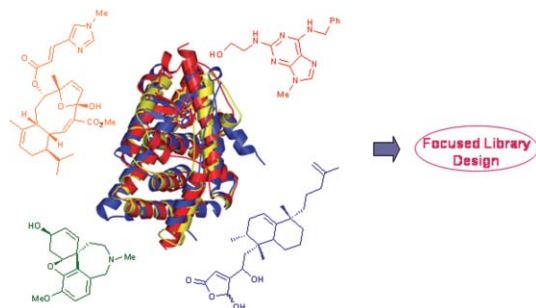
The current impact and future potential of genomics on cancer drug development is discussed. This second golden era of cancer drug development is now leading to personalized molecular therapeutics.



Functional gene-discovery systems based on libraries of hammerhead and hairpin ribozymes and short hairpin RNAs

Masayuki Sano, Yoshio Kato and Kazunari Taira*

Ribozyme-based and short hairpin RNA-based gene-discovery systems and their advantages over other methods for the identification of functional genes within the human genome are discussed.



Design of compound libraries based on natural product scaffolds and protein structure similarity clustering (PSSC)

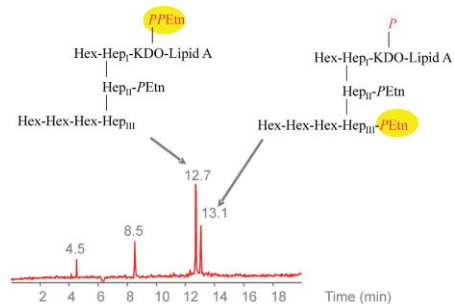
Rengarajan Balamurugan, Frank J. Dekker and Herbert Waldmann*

Natural product inspired library design in conjunction with protein structure similarity clustering provides increased hit rates in focused compound libraries which may find promising applications in drug discovery and chemical genomics approaches.

Electrophoretic and mass spectrometric strategies for profiling bacterial lipopolysaccharides

Jianjun Li,* Andrew D. Cox, Derek W. Hood, Elke K. H. Schweda, E. Richard Moxon and James C. Richards

The CE-MS analysis of LPS from *Haemophilus influenzae* strain 375.1 revealed the presence of two isoforms varying by the location of the phosphoethanolamine groups on the core structure.

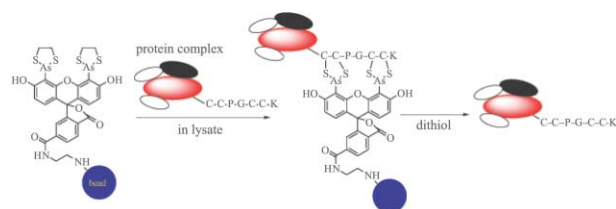


COMMUNICATION

One-step, non-denaturing isolation of an RNA polymerase enzyme complex using an improved multi-use affinity probe resin

M. Uljana Mayer,* Liang Shi and Thomas C. Squier

Isolation of intact protein complexes using a bisarsenical affinity reagent on a glass support permits the rapid identification of protein components by mass spectrometry.

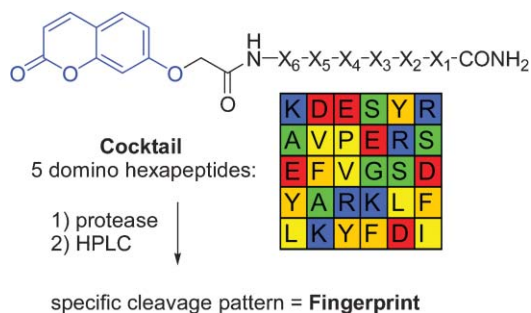


PAPERS

Protease profiling using a fluorescent domino peptide cocktail

Yang Yongzheng and Jean-Louis Reymond*

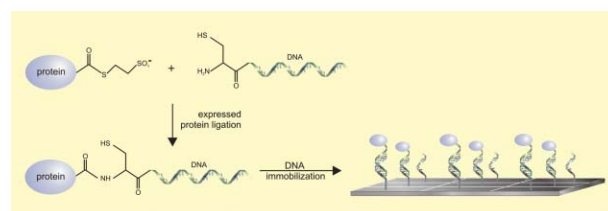
A cocktail of five coumarin-labeled hexapeptides with a domino sequence arrangement provides specific cleavage patterns allowing the functional identification of various proteases in a single HPLC assay.



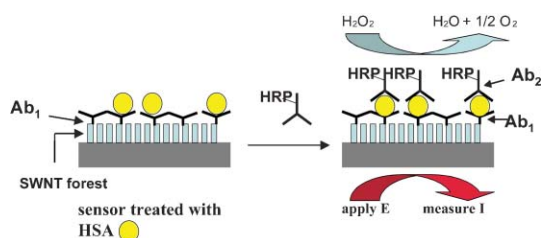
Synthesis of covalent DNA-protein conjugates by expressed protein ligation

Marina Lovrinovic, Mark Spengler, Carl Deutsch and Christof M. Niemeyer*

Efficient and site-specific covalent coupling of DNA oligomers and recombinant proteins is achieved by expressed protein ligation. The resulting conjugates, which retain their full biological activity, are versatile molecular tools.



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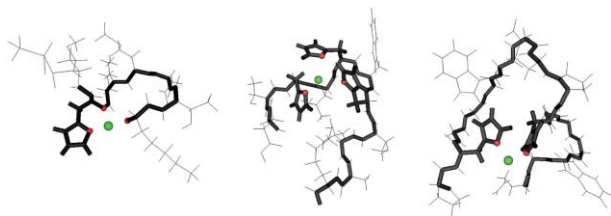


Protein immunosensor using single-wall carbon nanotube forests with electrochemical detection of enzyme labels

Xin Yu, Sang Nyon Kim, Fotios Papadimitrakopoulos* and James F. Rusling*

Vertically aligned single-wall carbon nanotube forests were used to fabricate enzyme-linked amperometric immunosensors featuring antibodies bioconjugated to nanotube ends. Using casein and detergent to minimize non-specific binding, a detection limit of 1 pmol mL^{-1} was achieved for human serum albumin.

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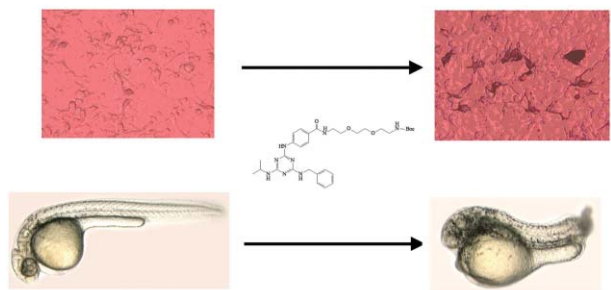


NMR studies on Cu(II)–peptide complexes: exchange kinetics and determination of structures in solution

Elena Gaggelli, Henryk Kozłowski, Daniela Valensin and Gianni Valensin*

Knowledge of structural and kinetic features of copper(II) strongly interacting with histidine-containing peptides taken from the human prion protein may shed light on relevant aspects of prion diseases. System-adapted NMR methods yield valuable geometrical restraints for determining structures in solution.

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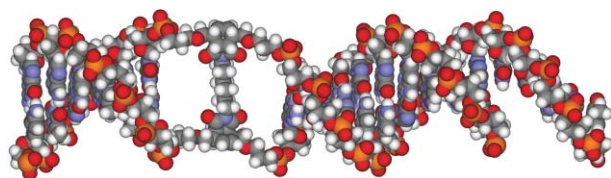


Identification of the F1F0 mitochondrial ATPase as a target for modulating skin pigmentation by screening a tagged triazine library in zebrafish

Da-Woon Jung, Darren Williams, Sonya M. Khersonsky, Tae-Wook Kang, Noushin Heidary, Young-Tae Chang and Seth J. Orlow*

A chemical probe identified from a zebrafish screening system has been successfully used in a forward chemical genetic approach to establish a link between the phenotype and the protein.

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Crosslinking of diene-modified DNA with bis-maleimides

Rolf Tona and Robert Häner*

Crosslinked oligonucleotide hybrids produced *via* the Diels–Alder reaction were shown to behave like two separate, hairpin-like structures, rather than like a single, continuous duplex.