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IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (28) 2929–3028 (2006)



Cover

See Jean-Marie Lehn, Andreas Herrmann *et al.*, page 2965. Chemistry in a washing machine: dynamic mixtures obtained by reversible reaction of perfumery aldehydes and ketones with acylhydrazides allow modulation of the evaporation of the volatiles from dry fabric. Image reproduced by permission of Barbara Levrand, Yves Ruff, Jean-Marie Lehn and Andreas Herrmann from *Chem. Commun.*, 2006, 2965.



Inside cover

See Ismael Cotte-Rodríguez and R. Graham Cooks, page 2968. A DESI source adapted to examine samples up to 3 metres from the mass spectrometer *via* a long ion transfer tube is used to ionize traces of RDX molecules in Composition C-4 by spraying reactant Cl^- ions onto the surface of the contaminated box forming stable adducts with RDX which are then transported back to the distant mass spectrometer, which is isolated from the sampling room *via* a protective shield. Image reproduced by permission of Ismael Cotte-Rodríguez and R. Graham Cooks from *Chem. Commun.*, 2006, 2968.

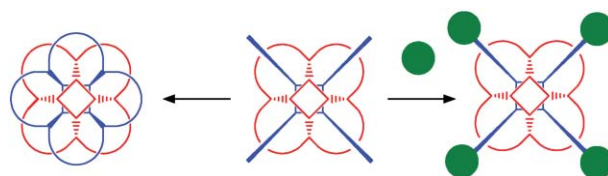
FEATURE ARTICLE

2941

Topologically novel multiple rotaxanes and catenanes based on tetraurea calix[4]arenes

Anca Bogdan, Yuliya Rudzevich, Myroslav O. Vysotsky and Volker Böhmer*

Hydrogen bonded dimers of tetraurea calix[4]arenes are used to preorganise alkenyl functions attached to the urea groups. Thus, a variety of multimacrocylic compounds including rotaxanes and catenanes were easily prepared by olefin metathesis.



COMMUNICATIONS

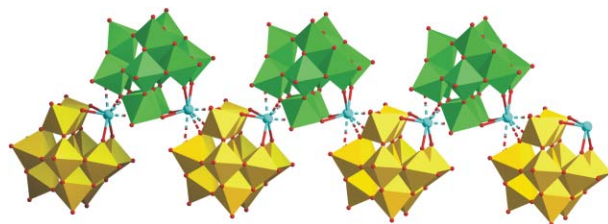
2953



One-dimensional silver(I) chain of lacunary α -Keggin anions

Helena I. S. Nogueira,* Filipe A. Almeida Paz,* Paula A. F. Teixeira and Jacek Klinowski

A novel chain-like silver polyoxotungstophosphate is formed when Ag^+ metal centres, exhibiting an unusual eight-coordination fashion, bridge a monolacunary $[\text{PW}_{11}\text{O}_{39}]^{7-}$ anion to four bridging μ_2 -oxygen atoms of a neighbouring lacunary α -Keggin anion.



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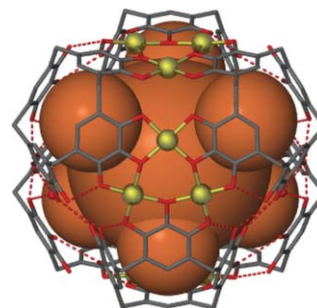
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2956

Hexameric C-alkylpyrogallol[4]arene molecular capsules sustained by metal-ion coordination and hydrogen bonds

Robert M. McKinlay, Praveen K. Thallapally and Jerry L. Atwood*

A large multicomponent nanospheroid structure consisting of six C-pentylpyrogallol[4]arene molecules and 12 Ga³⁺ metal-ions which in turn encloses 1150 Å³ of chemical space is reported.

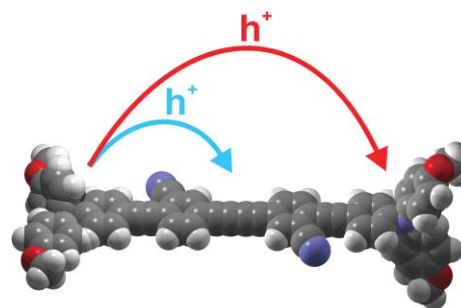


2959

Mulliken–Hush analysis of a bis(triarylamine) mixed-valence system with a N⋯N distance of 28.7 Å

Alexander Heckmann, Stephan Amthor and Christoph Lambert*

What is the largest redox centre separation for which the charge transfer behaviour of a mixed valence compound can be investigated by a Mulliken–Hush analysis? This problem is addressed by the analysis of the NIR transitions of a bis(triarylamine) radical cation with an electron deficient bridge unit.

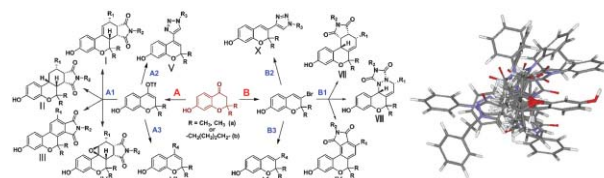


2962

Concise and diversity-oriented synthesis of novel scaffolds embedded with privileged benzopyran motif

Sung Kon Ko, Hwan Jong Jang, Eunha Kim and Seung Bum Park*

A branching DOS strategy for an unbiased natural product-like library with embedded privileged benzopyran motif was established to provide complexity and diversity of resulting heterocycles. The importance of skeletal diversity conducted on a privileged substructure was demonstrated through biological evaluation.

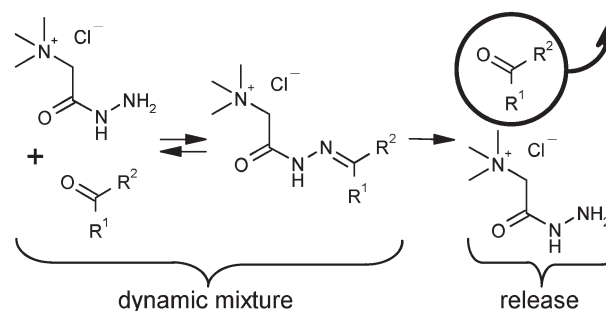


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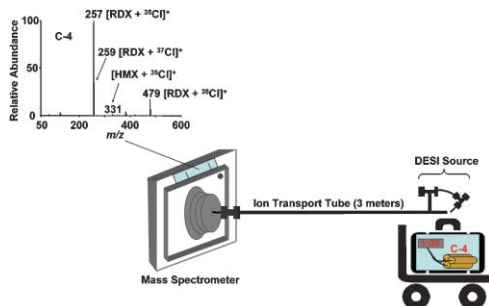
Controlled release of volatile aldehydes and ketones by reversible hydrazone formation – “classical” profragrances are getting dynamic

Barbara Levrant, Yves Ruff, Jean-Marie Lehn* and Andreas Herrmann*

Dynamic mixtures obtained by reversible acylhydrazone formation were found to be efficient in controlling the evaporation of highly volatile fragrance aldehydes and ketones from solid surfaces.



2968

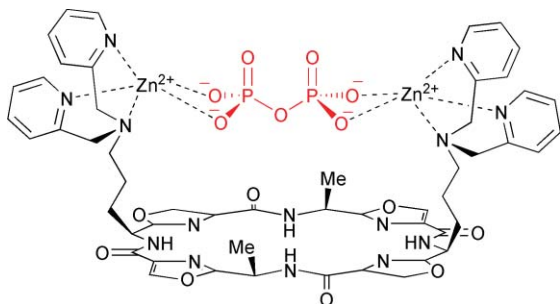


Non-proximate detection of explosives and chemical warfare agent simulants by desorption electrospray ionization mass spectrometry

Ismael Cotte-Rodríguez and R. Graham Cooks*

Desorption electrospray ionization (DESI) is used for the selective and sensitive detection of trace amounts of explosives and a chemical warfare agent simulant from ambient surfaces remote (1 to 3 meters) from the mass spectrometer.

2971

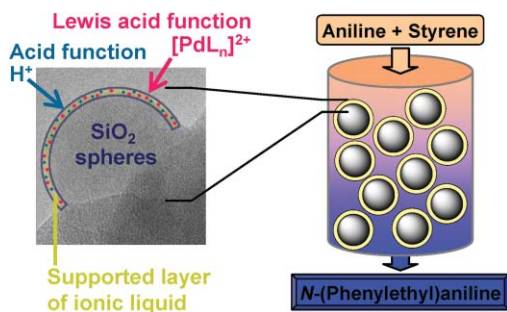


Selective recognition of pyrophosphate in water using a backbone modified cyclic peptide receptor

Matthew J. McDonough, Aaron J. Reynolds, Wee Yu Gladys Lee and Katrina A. Jolliffe*

A cyclic peptide based receptor, bearing two dipicolylamino arms complexed to zinc(II) ions, binds pyrophosphate ions with high affinity and selectivity in aqueous solution as determined using an indicator displacement assay.

2974

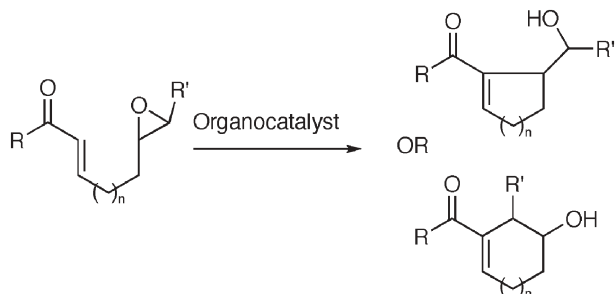


Markownikoff and *anti*-Markownikoff hydroamination with palladium catalysts immobilized in thin films of silica supported ionic liquids

Oriol Jimenez, Thomas E. Müller,* Carsten Sievers, Andreas Spirkel and Johannes A. Lercher

Novel bi-functional catalysts combining soft Lewis acidic and strong Brønsted acidic functions provided exceptional catalytic activity for the addition of aniline to styrene.

2977



New directions for the Morita–Baylis–Hillman reaction; homologous aldol adducts *via* epoxide opening

Marie E. Krafft* and James A. Wright

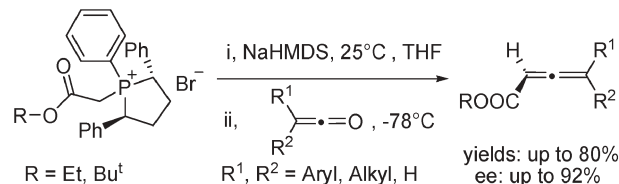
Under trialkylphosphine catalyzed Morita–Baylis–Hillman reaction conditions, epoxides react with enones to give rise to homologous aldol adducts.

2980

Enantioselective synthesis of allenic esters *via* an ylide route

Chuan-Ying Li, Xiu-Li Sun, Qing Jing and Yong Tang*

Pseudo- C_2 -symmetric chiral phosphorus ylides have been designed and synthesized for the enantioselective preparation of allenic esters, and up to 92% ee has been achieved.

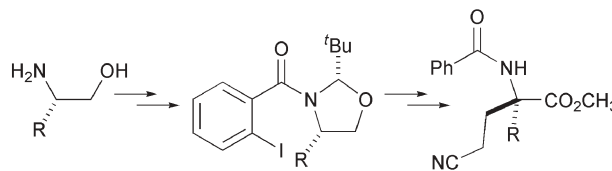


2983

A general route to protected quaternary α -amino acids from β -amino alcohols *via* a stereocontrolled radical approach

Mark E. Wood,* Mark J. Penny, Jenny S. Steere, Peter N. Horton, Mark E. Light and Michael B. Hursthouse

A radical-based approach facilitates the highly stereocontrolled functionalisation of β -amino alcohols, opening up a new, generally applicable methodology for the preparation of quaternary α -amino acids.

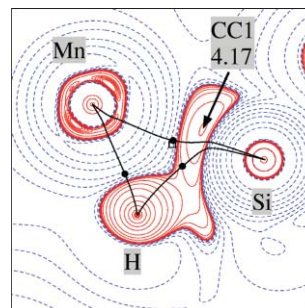


2986

Elucidation of the bonding in $\text{Mn}(\eta^2\text{-SiH})$ complexes by charge density analysis and T_1 NMR measurements: asymmetric oxidative addition and anomeric effects at silicon

Wolfgang Scherer,* Georg Eickerling, Maxim Tafipolsky, G. Sean McGrady,* Peter Sirsch and Nicholas P. Chatterton

Charge density analysis of $\text{Mn}(\eta^2\text{-SiH})$ complexes reveals an asymmetric oxidative addition controlled by the substitution pattern at the silicon centre, and in particular by the ligand *trans* to the η^2 -bound SiH moiety.

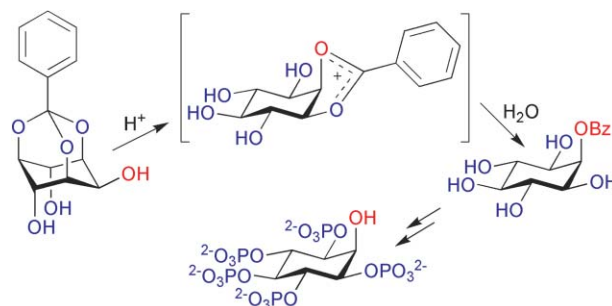


2989

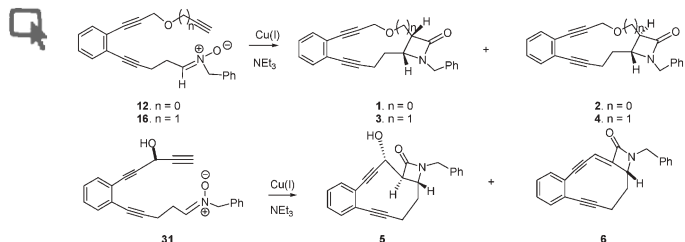
Regioselective hydrolysis of *myo*-inositol 1,3,5-orthobenzoate *via* a 1,2-bridged 2'-phenyl-1',3'-dioxolan-2'-ylium ion provides a rapid route to the anticancer agent $\text{Ins}(1,3,4,5,6)\text{P}_5$

Himali Y. Godage, Andrew M. Riley, Timothy J. Woodman and Barry V. L. Potter*

Acid hydrolysis of *myo*-inositol 1,3,5-orthobenzoate leads, unexpectedly, to 2-*O*-benzoyl-*myo*-inositol, the key precursor for a highly efficient synthesis of *myo*-inositol 1,3,4,5,6-pentakisphosphate.



2992

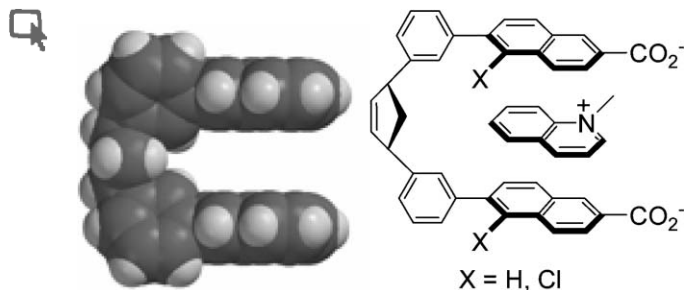


A novel synthesis of β -lactam fused cyclic enediynes by intramolecular Kinugasa reaction

Runa Pal and Amit Basak*

A general synthetic route to β -lactam-fused enediynes by intramolecular Kinugasa reaction has been successfully developed. The method has widened the scope of Kinugasa reaction in the synthesis of sensitive systems like the one described in this communication.

2995

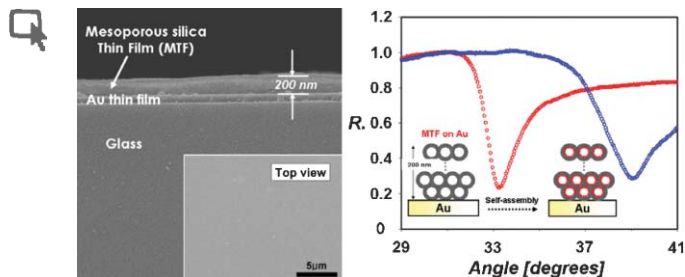


A modular molecular tweezer designed using CAVEAT

Haidong Huang and Dale G. Drueckhammer*

A computer-guided approach has been used to design a novel molecular tweezer based on a simple highly modular structure. Binding affinity to an aromatic guest determined by ¹H NMR spectroscopy is similar to that of other aryl group receptors.

2998



Mesoporous silica thin films as a spatially extended probe of interfacial electric fields for amplified signal transduction in surface plasmon resonance spectroscopy

Taewook Kang, Seogil Oh, Surin Hong, Jungwoo Moon and Jongheop Yi*

A new simpler concept about the signal amplification of surface plasmon resonance (SPR) that is based on the utilization of mesoporous silica thin films is demonstrated.

3001



EDG = OH, OMe, OCH₂O, SMe, NH₂, NMe₂
X = Cl, F, OMs, OTf, OPO₃Et₂

Convenient synthesis of electron-donating substituted benzonitriles by photolysis of phenyl halides and esters

Valentina Dichiarante, Maurizio Fagnoni* and Angelo Albini

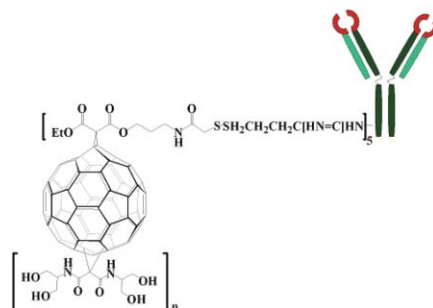
A novel metal-free synthesis of electron-rich benzonitriles through an ArS_N1 pathway has been accomplished by the reaction of photogenerated (from phenyl halides or esters) triplet phenyl cations with cyanide ions.

3004

Fullerene (C₆₀) immunoconjugates: interaction of water-soluble C₆₀ derivatives with the murine anti-gp240 melanoma antibody

Jared M. Ashcroft, Dmitri A. Tsyboulski, Keith B. Hartman, Tatiana Y. Zakharian, John W. Marks, R. Bruce Weisman, Michael G. Rosenblum and Lon J. Wilson*

The first fullerene (C₆₀) immunoconjugates have been prepared and characterized as an initial step toward the development of fullerene immunotherapy (FIT).

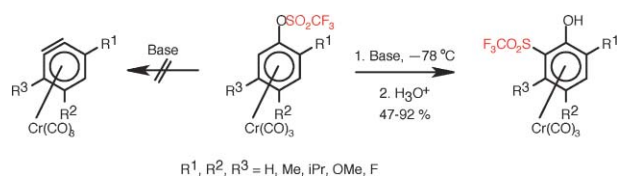


3007

Unanticipated formation of *ortho*-sulfone substituted phenols by anionic thia-Fries rearrangement of (aryl triflate)tricarboxylchromium complexes

Zhirong Zhao, Josef Messinger, Uwe Schön, Rudolf Wartchow and Holger Butenschön*

Attempts to generate (benzyne)tricarboxylchromium complexes by triflic acid elimination unexpectedly resulted in *ortho*-(trifluoromethylsulfonyl)phenol complex formation as a result of an anionic thia-Fries rearrangement.

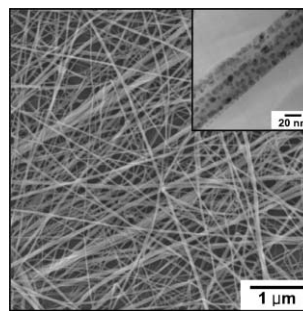


3010

One-step fabrication of silver nanoparticle embedded polymer nanofibers by radical-mediated dispersion polymerization

Hyeyoung Kong and Jyongsik Jang*

Silver nanoparticle embedded PVA–PMMA nanofibers were fabricated by one-step radical-mediated dispersion polymerization using AIBN as a reductant of silver ions.

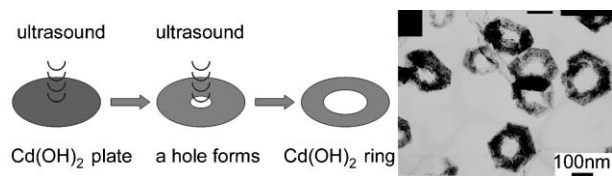


3013

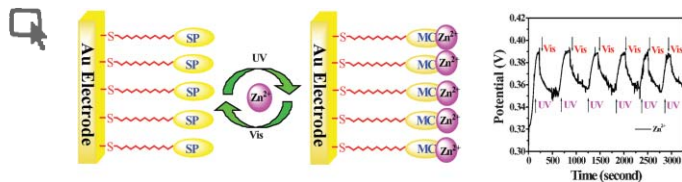
Fabrication of Cd(OH)₂ nanorings by ultrasonic chiselling on Cd(OH)₂ nanoplates

Jian-Jun Miao, Rui-Ling Fu, Jian-Min Zhu, Ke Xu, Jun-Jie Zhu* and Hong-Yuan Chen

Cd(OH)₂ nanorings were successfully fabricated from Cd(OH)₂ nanoplates by ultrasonic chiselling, a unique effect of the sonochemical process that has never been reported before.



3016

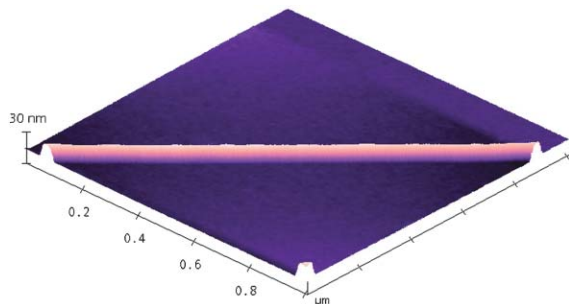


Photomodulation of the electrode potential of a photochromic spiropyran-modified Au electrode in the presence of Zn^{2+} : a new molecular switch based on the electronic transduction of the optical signals

Guoyong Wen, Jie Yan, Yucheng Zhou, Deqing Zhang,* Lanqun Mao* and Daoben Zhu*

The electrode potential of a photochromic spiropyran-modified Au electrode is reversibly modulated by UV/visible light irradiation in the presence of Zn^{2+} . A new molecular switch and an “AND” logic gate based on this optical signal transduction are established.

3019



Study and characterization of tobacco mosaic virus head-to-tail assembly assisted by aniline polymerization

Zhongwei Niu, Michael Bruckman, Venkata S. Kotakadi, Jinbo He, Todd Emrick, Thomas P. Russell, Lin Yang and Qian Wang*

One-dimensional composite nanofibres with narrow dispersity, high aspect ratio and high processibility were fabricated by head-to-tail self-assembly of rod-like tobacco mosaic virus assisted by aniline polymerization.

3022

Debangshu Chaudhuri and D. D. Sarma

Blue emitting polyaniline

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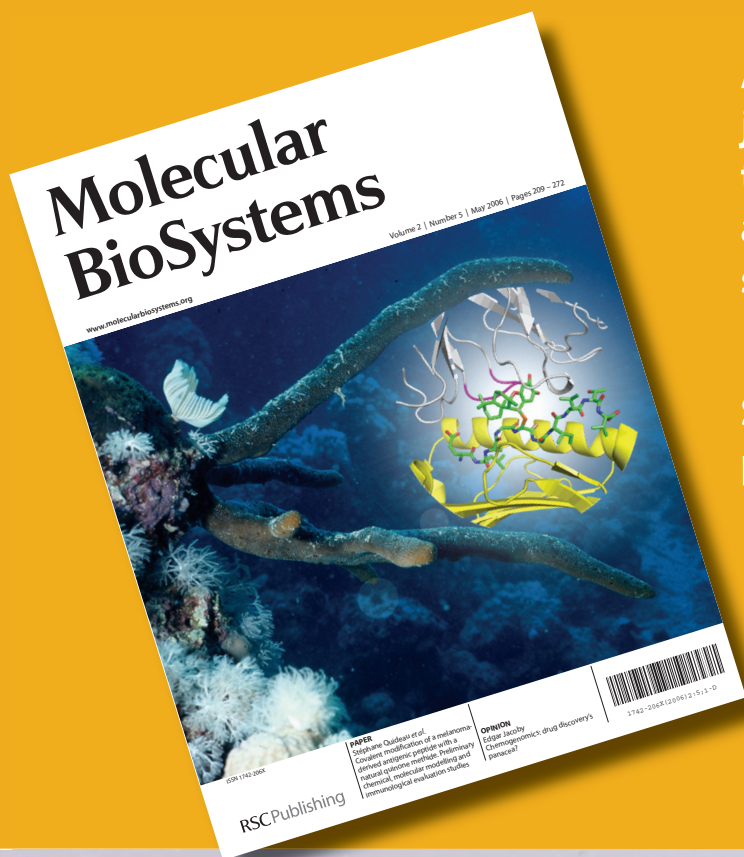
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