

# ChemComm

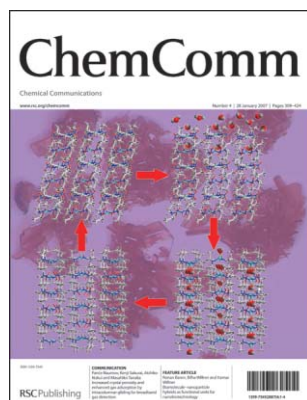
Chemical Communications

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## IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (4) 309–424 (2007)



### Cover

See Panče Naumov *et al.*, page 347.  
Asymmetric coordinatively unsaturated units glide back and forth to open structural channels for accommodation of small gaseous molecules. Image reproduced by permission of Panče Naumov, Kenji Sakurai, Akihiko Nukui and Masahiko Tanaka from *Chem. Commun.*, 2007, 347.



### Inside cover

See Piero Sozzani *et al.*, page 350.  
 $^{129}\text{Xe}$  HP NMR resonance can be fine-tuned to a given radiofrequency by turning a porous single-crystal as the tuning knob. Image reproduced by permission of Angiolina Comotti, Silvia Bracco, Lisa Ferretti, Michele Mauri, Roberto Simonutti and Piero Sozzani from *Chem. Commun.*, 2007, 350.

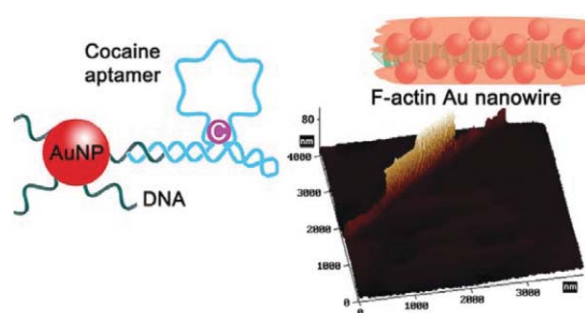
## FEATURE ARTICLES

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### Biomolecule–nanoparticle hybrids as functional units for nanobiotechnology

Ronan Baron, Bilha Willner and Itamar Willner\*

Biomolecule–nanoparticle hybrid systems provide unique assemblies for the electrical or optical biosensing, and for the fabrication of nanowires and nanodevices.

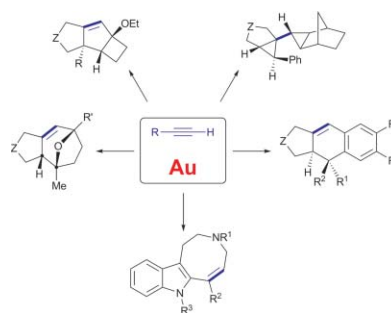


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### Molecular diversity through gold catalysis with alkynes

Eloísa Jiménez-Núñez and Antonio M. Echavarren\*

We highlight the wide molecular diversity that can be achieved using gold-catalysed transformations, in particular with regard to the formation of C–C bonds.



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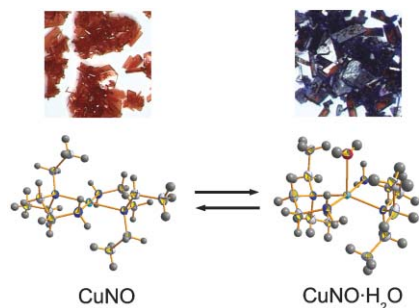
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### Increased crystal porosity and enhanced gas adsorption by intracolumnar gliding for broadband gas detection

Panče Naumov,\* Kenji Sakurai, Akihiko Nukui and Masahiko Tanaka

A new three-level structural approach based on anion-induced intracolumnar gliding of stacked coordinatively unsaturated units is described for design of metal–organic crystals which exhibit concentration- and gas-specific adsorption of small molecules.

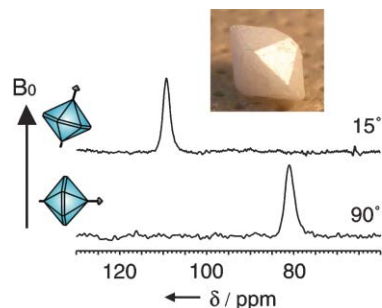


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### A single-crystal imprints macroscopic orientation on xenon atoms

Angiolina Comotti, Silvia Bracco, Lisa Ferretti, Michele Mauri, Roberto Simonutti and Piero Sozzani\*

A porous single-crystal collects xenon atoms from the gas phase and orients them macroscopically, as highlighted by hyperpolarized xenon NMR.

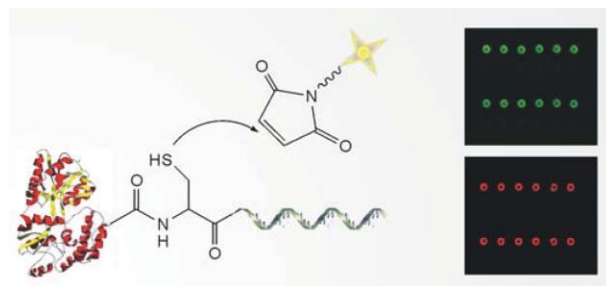


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### Site-specific labeling of DNA–protein conjugates by means of expressed protein ligation

Marina Lovrinovic, Ljiljana Fruk, Hendrik Schröder and Christof M. Niemeyer\*

Site-specific bioconjugation of protein thioesters with a DNA oligonucleotide was achieved by Expressed Protein Ligation (EPL) and the new thiol group formed upon EPL in the conjugate was selectively coupled with small molecule labels using maleimide chemistry.

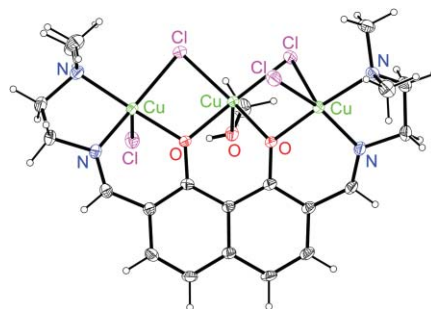


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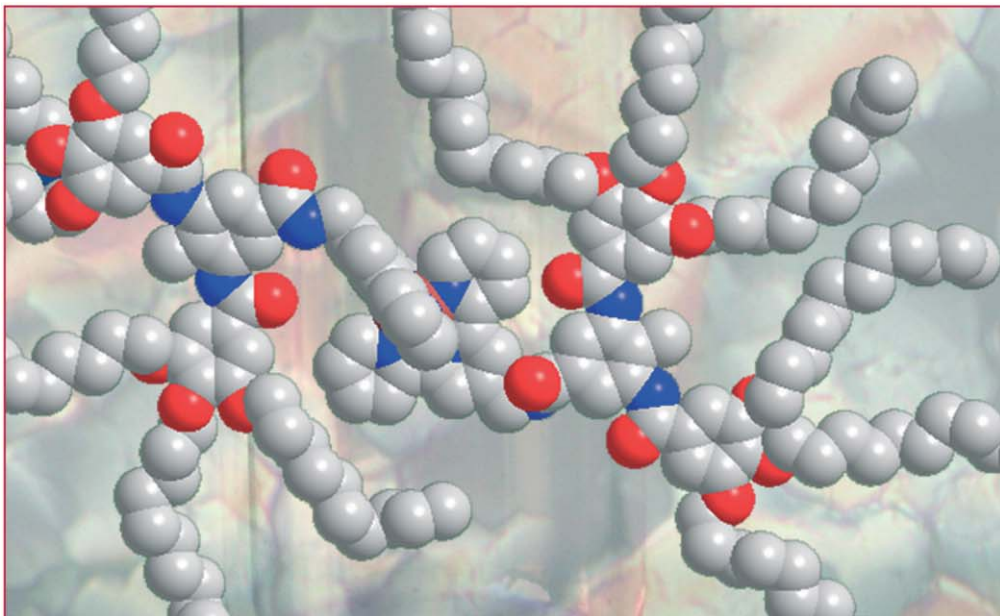
### A trinucleating ligand based on 1,8-naphthalenediol: synthesis, structural and magnetic properties of a linear Cu<sup>II</sup>Cu<sup>II</sup>Cu<sup>II</sup> complex

Thorsten Glaser,\* Ioannis Liratzis, Roland Fröhlich and Thomas Weyhermüller

The building block 2,7-diformyl-1,8-naphthalenediol has been used for the extension of dinucleating Robson-type ligands to the first trinucleating derivative as demonstrated by the synthesis, structural and magnetic characterization of the trinuclear Cu<sup>II</sup>Cu<sup>II</sup>Cu<sup>II</sup> complex shown.







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*Benoît Champin, Valérie Sartor, Jean-Pierre Sauvage (France)*

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*Laurent Vial, Jeremy K. M. Sanders, Sijbren Otto (UK)*

**The first total synthesis of aeruginosamide**

*Zhiyong Chen, Tao Ye (China)*

**Molecular knots, links, and fabrics: prediction of existence and suggestion of a synthetic route**

*Dirk Andrae (Germany)*

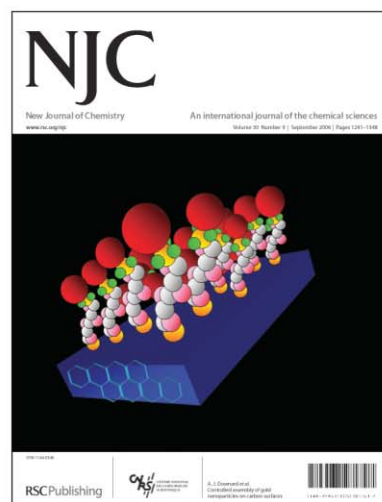
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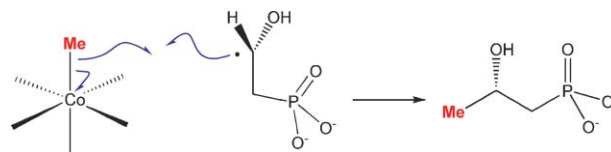
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### New insight into the mechanism of methyl transfer during the biosynthesis of fosfomicin

Ryan D. Woodyer, Gongyong Li, Huimin Zhao\* and Wilfred A. van der Donk\*

Hydroxyethylphosphonate is a required intermediate in fosfomicin biosynthesis.

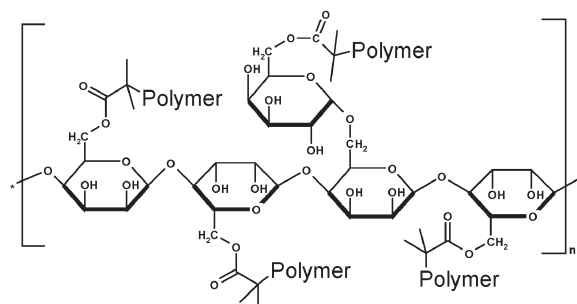


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### Synthesis of well-defined Locust Bean Gum-graft-copolymers using ambient aqueous atom transfer radical polymerisation

Steven P. Rannard,\* Susanne H. Rogers and Robert Hunter

The first atom transfer radical graft copolymerisation at ambient temperature in water from a soluble polysaccharide is demonstrated for a range of monomer types.

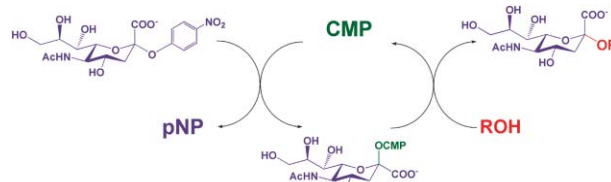


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### Alternative donor substrates for inverting and retaining glycosyltransferases

Luke L. Lairson, Warren W. Wakarchuk and Stephen G. Withers\*

Expensive nucleotide sugar substrates for glycosyltransferases can be replaced with aryl glycosides of the opposite anomeric configuration if catalytic amounts of nucleotide are added.

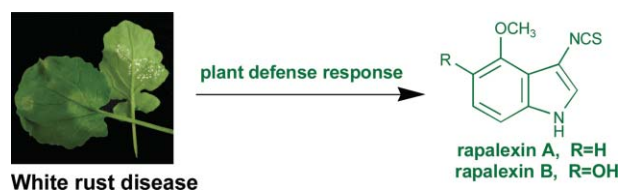


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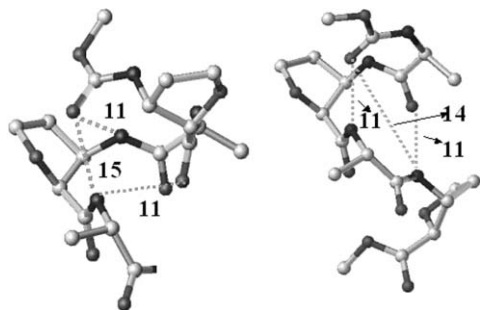
### The first naturally occurring aromatic isothiocyanates, rapalexins A and B, are cruciferous phytoalexins

M. Soledade C. Pedras,\* Qing-An Zheng and Ravi S. Gadagi

Rapalexins A and B display remarkable inhibitory activity against the white rust pathogen, a very damaging pest of crucifers.



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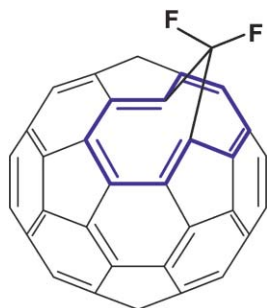


### Formation of left-handed helices in hybrid peptide oligomers with *cis* $\beta$ -sugar amino acid and L-Ala as building blocks

Bharatam Jagadeesh,\* Anabathula Prabhakar, Ganti Dattatreya Sarma, Srivari Chandrasekhar,\* Gudise Chandrashekar, Marepally Srinivasa Reddy and Bulusu Jagannadh\*

A new class of short hybrid peptide oligomers consisting of alternating L-Ala and *cis*- $\beta$ -furanoid sugar amino acid residues are reported, which exhibit the co-existence of left-handed 11- and 14/15-helical conformations.

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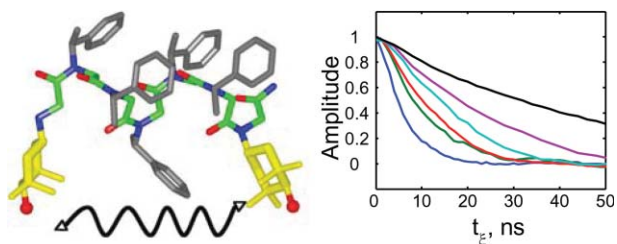


### Synthesis and characterization of difluoromethylene-homo[60]fullerene, $C_{60}(CF_2)$

Anna S. Pimenova, Andrey A. Kozlov, Alexey A. Goryunkov, Vitaliy Yu. Markov, Pavel A. Khavrel, Stanislav M. Avdoshenko, Ilya N. Ioffe, Sergey G. Sakharov, Sergey I. Troyanov and Lev N. Sidorov\*

Homo[60]fullerene  $C_{60}(CF_2)$  with a cleaved [6,6]-bond has been obtained by reacting  $C_{60}$  with  $CF_2ClCOONa$ . Its molecular structure has been elucidated by means of NMR, IR, and UV/Vis spectroscopic studies and DFT calculations.

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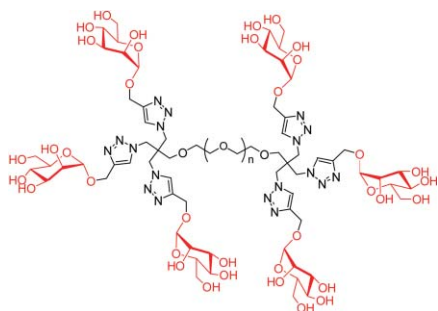


### Characterizing the structure and dynamics of folded oligomers: Pulsed ESR studies of peptoid helices

Aaron T. Fafarman, Peter P. Borbat, Jack H. Freed and Kent Kirshenbaum\*

Pulsed electron spin resonance spectroscopy is applied to elucidate the structure and dynamics of helical N-substituted glycine "peptoids" incorporating nitroxide spin probes in the oligomer sidechains.

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### Tri- and hexavalent mannoside clusters as potential inhibitors of type 1 fimbriated bacteria using pentaerythritol and triazole linkages

Mohamed Touaibia, Tze Chieh Shiao, Alex Papadopoulos, Jonathan Vaucher, Qingan Wang, Karima Benhamioud and René Roy\*

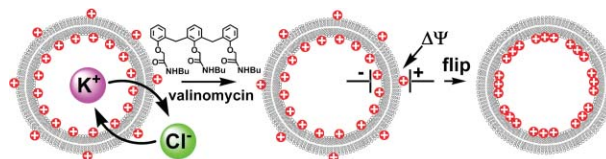
Several oligomannoside clusters showing a hundred-fold increase in affinities toward *E. coli* were synthesized by Cu(I)-catalyzed [1,3]-dipolar cycloadditions using pentaerythritol scaffolds bearing either alkyne or azide functionalities.

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### Towards improved gene delivery: Flip of cationic lipids in highly polarized liposomes

Richard G. Uhl, II, Amalia Stevenson and Vladimir Sidorov\*

Hyperpolarization of cationic liposomes by a concerted action of  $K^+$ -transporter valinomycin and  $Cl^-$ -transporter triphenoxyacetamide improves their stability in the presence of human serum albumin.

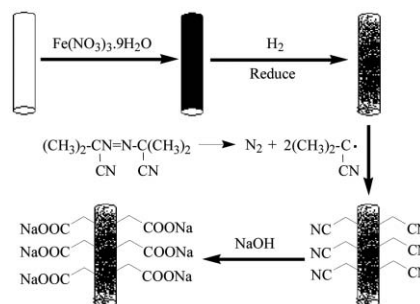


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### Magnetic Fe nanoparticle functionalized water-soluble multi-walled carbon nanotubes towards the preparation of sorbent for aromatic compounds removal

Jun Jin, Rong Li, Huanling Wang, Hangning Chen, Kun Liang and Jiantai Ma\*

Magnetic Fe nanoparticle functionalized water-soluble multi-walled carbon nanotubes (MWNTs) were prepared, characterized and used for the removal of aromatic compounds in water and re-use.

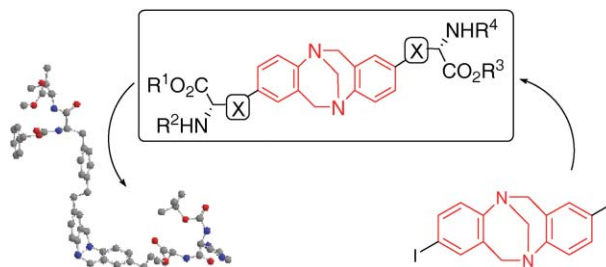


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### $\alpha$ -Amino acid Tröger base derivatives, possible conformationally restricted scaffolds?

Sean P. Bew,\* Laurent Legentil, Vincent Scholier and Sunil V. Sharma

The first synthesis of innovative  $\alpha$ -amino acid Tröger base derivatives is reported and their application as conformationally restricted scaffolds is proposed.

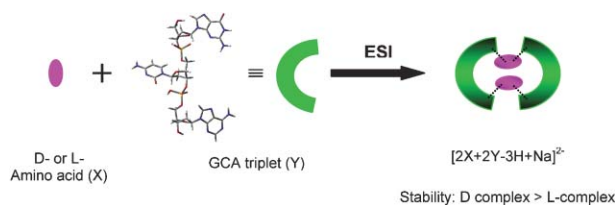


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### Chiral discrimination of $\alpha$ -amino acids by the DNA triplet GCA

Maddula Ravikumar, Sripadi Prabhakar and Mariappanadar Vairamani\*

This communication reports for the first time on the use of a DNA triplet as a selector for the chiral discrimination of amino acids by mass spectrometry.





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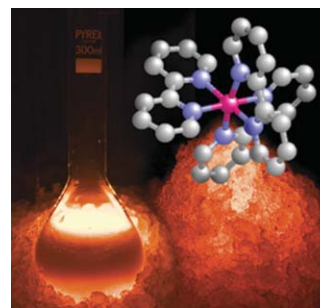


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### Tris(2,2'-bipyridyl)ruthenium(II) chemiluminescence enhanced by silver nanoparticles

Bree A. Gorman, Paul S. Francis, Dave E. Dunstan and Neil W. Barnett\*

Chemiluminescence from the reaction between tris(2,2'-bipyridyl)ruthenium(II), cerium(IV) and citrate is enhanced by silver ions, due to the formation of silver–citrate complexes and citrate-capped silver nanoparticles.

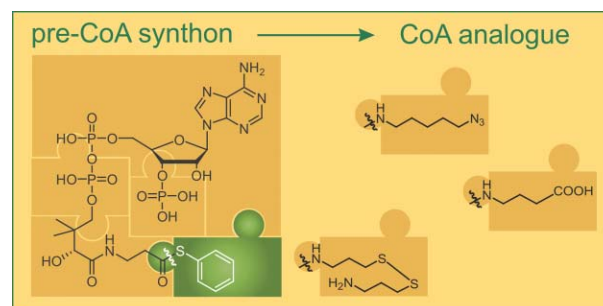


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### One-pot preparation of coenzyme A analogues via an improved chemo-enzymatic synthesis of pre-CoA thioester synthons

Marianne van Wyk and Erick Strauss\*

We present an improved one-pot synthesis of CoA analogues by aminolysis of a single activated thioester precursor, a pre-CoA synthon, which is prepared by biotransformation of a pantothenate thioester using the CoA biosynthetic enzymes.

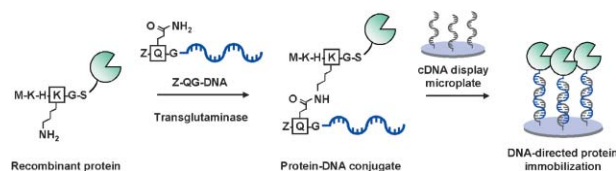


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### An enzymatic method for site-specific labeling of recombinant proteins with oligonucleotides

Jo Tominaga, Yoshinori Kemori, Yusuke Tanaka, Tatsuo Maruyama, Noriho Kamiya\* and Masahiro Goto

DNA was site-specifically conjugated to a substrate peptide of microbial transglutaminase fused to the N- or C-terminus of target proteins without the loss of the proteins' functions of interest.

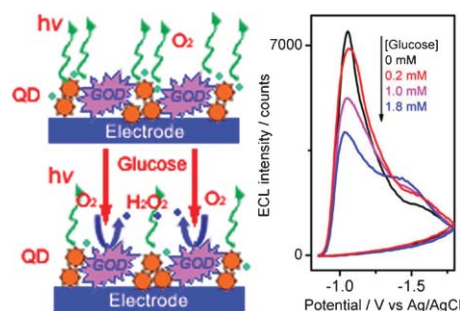


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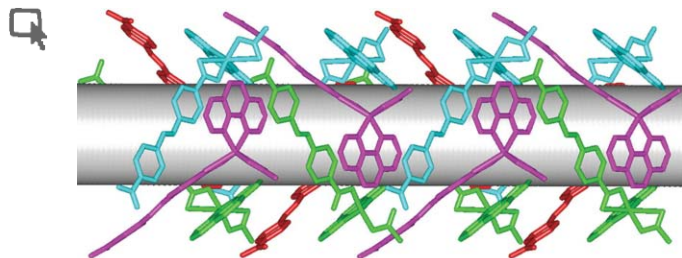
### Enzyme–quantum dots architecture for highly sensitive electrochemiluminescence biosensing of oxidase substrates

Hui Jiang and Huangxian Ju\*

This work proposes a simple strategy for the fabrication of the first biosensor based on the intrinsic electrochemiluminescence of quantum dots coupled with an enzymatic reaction.



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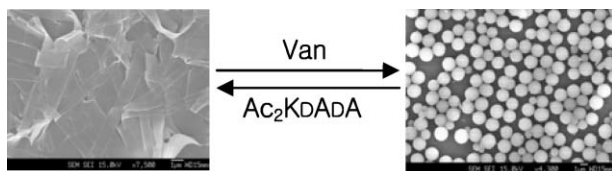


### Unprecedented 3D entanglement of 1D zigzag coordination polymers leading to a robust microporous framework

Ai-Ling Cheng, Na Liu, Yan-Feng Yue, Yong-Wen Jiang, En-Qing Gao,\* Chun-Hua Yan and Ming-Yuan He

One-dimensional zigzag coordination chains in four different directions are hierarchically entangled to generate an unprecedented 3D interwoven framework, which exhibits permanent porosity and guest selectivity.

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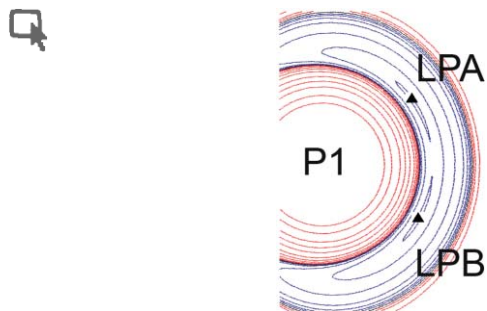


### Vancomycin-induced morphological transformation of self-assembled amphiphilic diacetylene supramolecules

Kun Ha Park, Ji-Seok Lee, Hyunwook Park, Eun-Hye Oh and Jong-Man Kim\*

Ribbon-shaped diacetylene supramolecules prepared with dipeptide-containing diacetylene PCDA-D-Ala-D-Ala **2** were converted to submicron-sized spheres in the presence of vancomycin. Addition of Ac-Lys(Ac)-D-Ala-D-Ala to microspheres resulted in the regeneration of ribbon-shaped morphologies.

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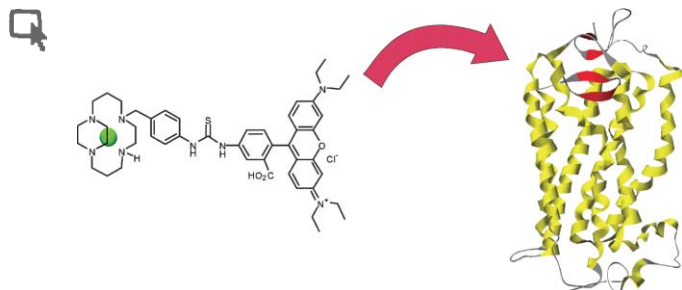


### The $P(bth)_2^-$ anion as a *Janus head* staple between lithium and manganese ( $bth = \text{benzothiazol-2-yl}, C_7H_4NS$ )

Thomas Stey, Julian Henn and Dietmar Stalke\*

$P(bth)_2^-$  is a site-selective *Janus head* ligand that coordinates a hard lithium cation and two soft  $CpMn(CO)_2$ -residues, mimicking a 4-electron phosphorus donor.

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### Fluorescent CXCR4 chemokine receptor antagonists: metal activated binding

Abid Khan, Jon D. Silversides, Leigh Madden, John Greenman and Stephen J. Archibald\*

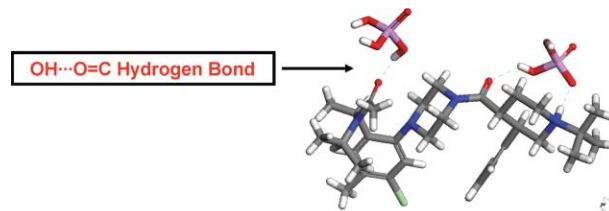
A novel rhodamine-azamacrocyclic conjugate has been synthesised that can be activated to bind to a specific cell surface receptor by complexation of a copper(II) ion.

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### Development of a pharmaceutical cocrystal of a monophosphate salt with phosphoric acid

Alex M. Chen,\* Martha E. Ellison,\* Andrey Peresyphkin, Robert M. Wenslow, Narayan Variankaval, Cecile G. Savarin, Theresa K. Natishan, David J. Mathre, Peter G. Dormer, Danielle H. Euler, Richard G. Ball, Zhixiong Ye, Yaling Wang and Ivan Santos

The first pharmaceutical cocrystal formed between an inorganic acid and an active pharmaceutical ingredient gives a stable crystalline and bioavailable solid dosage form.



# Chemistry and Medicines

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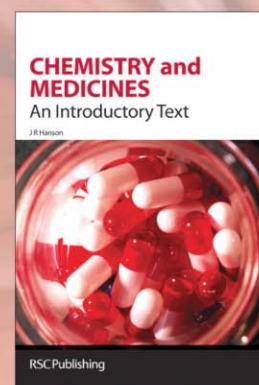
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