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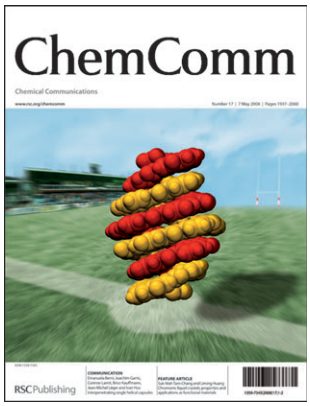
IN THIS ISSUE

ISSN 1359–7345 CODEN CHCOFS (17) 1937–2060 (2008)



Cover

See Ivan Huc *et al.*, pp. 1968–1970.
A double helical molecule with a rugby ball shape. Yellow and red are the colors of Cambridge, host city of ChemComm Editorial Office. Image by Mr Xavier Bourdil. Image reproduced by permission of Emanuela Berni, Joachim Garric, Corinne Lamit, Brice Kaumann, Jean-Michel Léger and Ivan Huc from *Chem. Commun.*, 2008, 1968.

CHEMICAL BIOLOGY

B33

Drawing together the research highlights and news from all RSC publications, *Chemical Biology* provides a 'snapshot' of the latest developments in chemical biology, showcasing newsworthy articles and significant scientific advances.

Chemical Biology

May 2008/Volume 3/Issue 5

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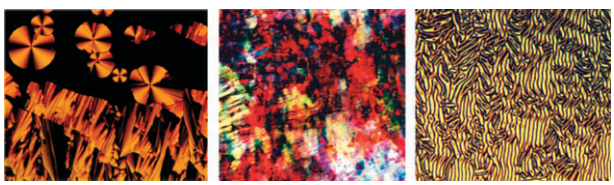
FEATURE ARTICLE



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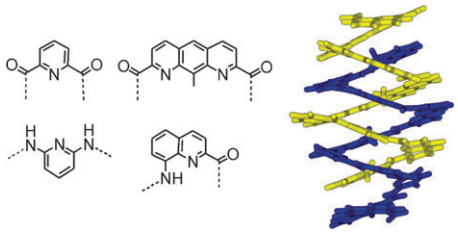
1968

Interpenetrating single helical capsules

Emanuela Berni, Joachim Garric, Corinne Lamit, Brice Kauffmann, Jean-Michel Léger and Ivan Huc*

Two helical capsules may interpenetrate to form a rugby ball shaped duplex in which each strand fill the hollow of the other strand.

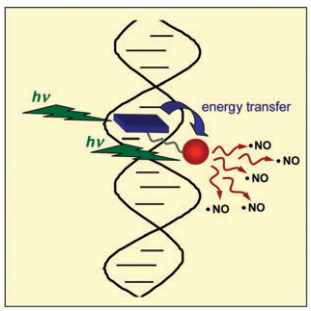


1971

Amplified nitric oxide photorelease in DNA proximity

Fiorella L. Callari and Salvatore Sortino*

A novel bichromophoric molecular system integrating a DNA intercalator and a NO photodonor allows the light-controlled delivery of NO nearby DNA and amplifies NO release *via* effective photoinduced energy transfer mechanism.

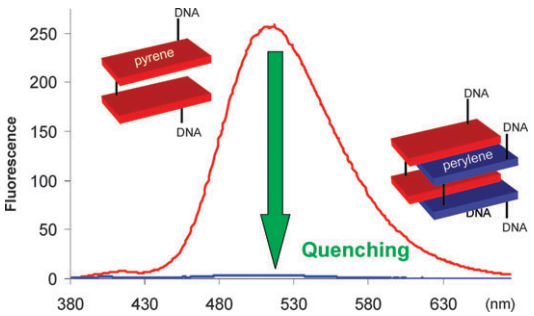


1974

Highly efficient quenching of excimer fluorescence by perylene diimide in DNA

Nicolas Bouquin, Vladimir L. Malinovskii and Robert Häner*

Perylene diimide (PDI) is described as a powerful fluorescence quencher. The excimer signal present in single stranded DNA containing adjacent pyrenes is completely suppressed upon duplex formation with a PDI modified complementary strand. The efficiency of the process is attributed, at least partly, to interstrand stacking of pyrene and PDI units.

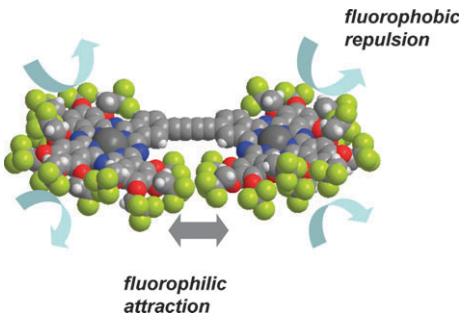


1977

Synthesis and properties of trifluoroethoxy-coated binuclear phthalocyanine

Hideyuki Yoshiyama, Norio Shibata,* Takefumi Sato, Shuichi Nakamura and Takeshi Toru

A genuine example of a non-aggregated highly fluorescent trifluoroethoxy-coated binuclear phthalocyanine is reported. Fluorophobic repulsion and fluorophilic attraction exist together in the molecule.



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Daejeon Convention Center
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Scientific Themes

- Discovery of New Reagents and Reactions
- Challenges in Natural Products Synthesis
- Prospects in Bioorganic Chemistry and Chemical Biology
- Visions in Organic Materials Research
- Events in Drug Process Development and Discovery

Invited Speakers (confirmed)

David Ager (USA)
Takuzo Aida (Japan)
Joe Armstrong (USA)
Carsten Bolm (Germany)
David E. Cane (USA)
Chien-Hong Cheng (Taiwan)
Jean M. J. Frechet (USA)
Tohru Fukuyama (Japan)
Samuel H. Gellman (USA)
Andrew D. Hamilton (USA)
Susumi Hatakeyama (Japan)
Minoru Isobe (Japan)
Alan Katritzky (USA)
Kyoung Soon Kim (USA)
Michael Kort (USA)
Michael J. Krische (USA)
James Leahy (USA)
Teck Peng Loh (Singapore)
Stephen F. Martin (USA)
Goverdhan Mehta (India)
Klaus Mullen (Germany)
Kazuhiko Nakatani (Japan)
Ian Paterson (UK)
Timothy Ramsey (USA)
Peter H. Seeberger (Switzerland)
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Chris Senanayake (USA)
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Brian M. Stoltz (USA)
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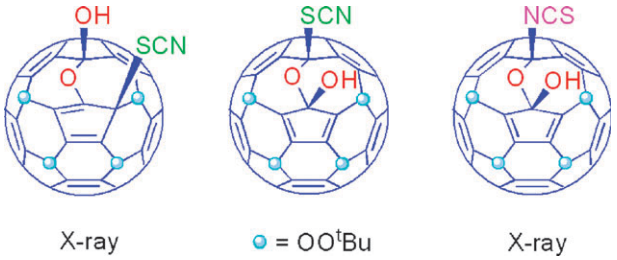
Keiji Tanino (Japan)
Kiyoshi Tomioka (Japan)
F. Dean Toste (USA)
Rajappa Vaidyanathan (USA)
Jurgen Wagner (Switzerland)
David R. Williams (USA)
Chi-Huey Wong (Taiwan)
Shigehiro Yamaguchi (Japan)
Dan Yang (Hong Kong)

1980

Controlled regio- and chemoselective addition of isothiocyanate to the dione moiety of a cage-opened fullerene-mixed peroxide derivative

Xiaobing Yang, Liangbing Gan* and Zheming Wang*

Lewis acids control the addition pattern of the ambident SCN group to the fullerene cage.

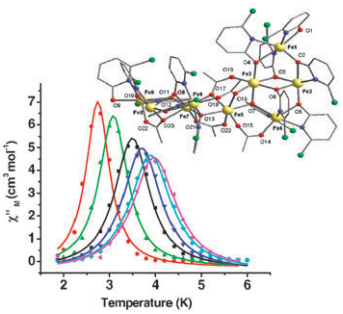


1983

A homospin iron(II) single chain magnet

Szymon W. Przybylak, Floriana Tuna,* Simon J. Teat and Richard E. P. Winpenny*

Synthetic, structural and magnetic studies of a new Fe(II) single chain magnet are reported.

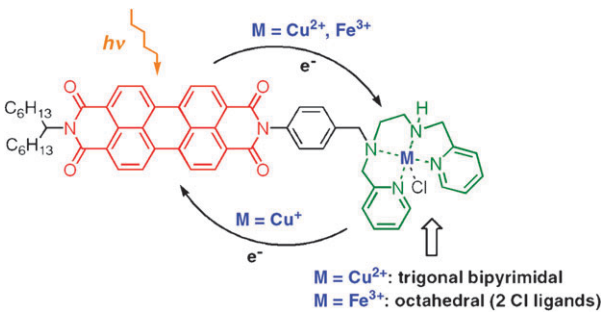


1986

Perylenediimide—metal ion dyads for photo-induced electron transfer

Katrine Qvortrup, Andrew D. Bond, Anne Nielsen, Christine J. McKenzie, Kristine Kilså* and Mogens Brøndsted Nielsen*

A novel perylene diimide incorporating a tetradentate ligand was synthesized and the possibility for photo-induced electron transfer to or from coordinated metal ions was investigated.

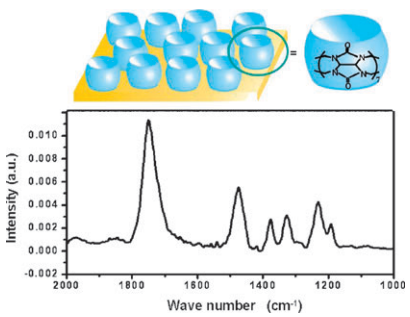


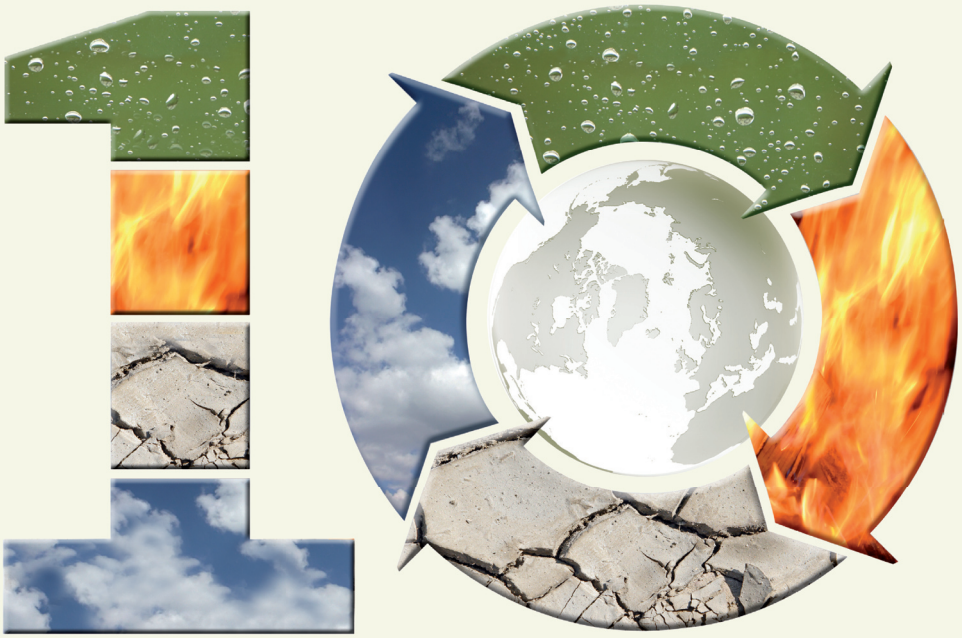
1989

A general and efficient method to form self-assembled cucurbit[*n*]uril monolayers on gold surfaces

Qi An, Guangtao Li,* Chengan Tao, Yan Li, Yiguang Wu and Weixia Zhang

A general protocol based on spontaneous adsorption of cucurbit[*n*]uril (CB[*n*]) molecules through a strong multivalence interaction between CB[*n*] and gold is described, by which the formation of self-assembled CB[*n*] monolayers on gold surfaces can be efficiently achieved.





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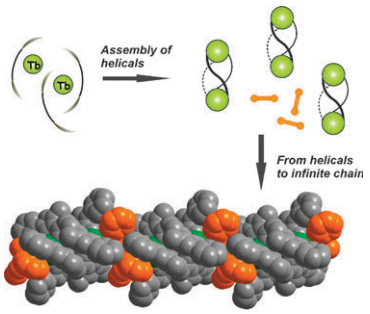
1992

First direct assembly of molecular helical complexes into a coordination polymer

Sergey N. Semenov,* Andrey Yu. Rogachev, Svetlana V. Eliseeva, Claudio Pettinari, Fabio Marchetti, Andrey A. Drozdov and Sergey I. Troyanov

Luminescent triple-stranded helicates, formed between Tb(III) ions and bis-acylpyrazolones, were directly assembled into a 1-D polymeric system.

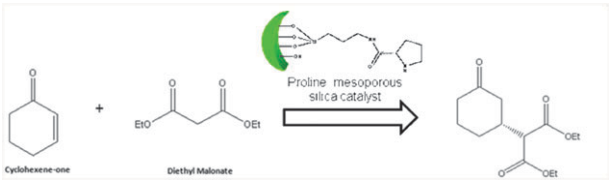


1995

Chiral enhancement in diethyl malonate addition by morphosynthesized L-proline mesoporous silica

Eko Adi Prasetyanto, Seung-Cheol Lee, Sung-Min Jeong and Sang-Eon Park*

L-Proline was immobilized onto mesoporous silica through direct synthesis method *via* morphosynthesis possessing short channels and plugs in the pore structure which provided chiral enhancement in the diethyl malonate addition reaction.

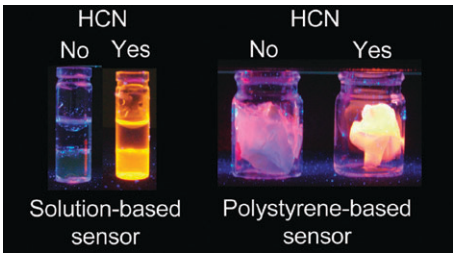


1998

Selective turn-on fluorescence detection of cyanide in water using hydrophobic CdSe quantum dots

Angeles Touceda-Varela, Emily I. Stevenson, José A. Galve-Gasión, David T. F. Dryden and Juan C. Mareque-Rivas*

The ability of 2,2′-bipyridine-bound copper(II) ions to quench the photoluminescence of hydrophobic CdSe quantum dots is used to create a novel, selective turn-on fluorescence cyanide sensor that works in solution and attached to polystyrene.

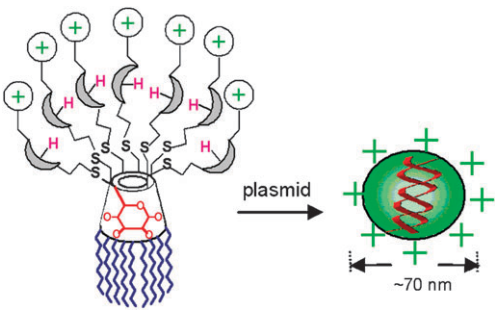


2001

Rational design of cationic cyclooligosaccharides as efficient gene delivery systems

Alejandro Díaz-Moscoso, Patricia Balbuena, Marta Gómez-García, Carmen Ortiz Mellet,* Juan M. Benito, Loïc Le Gourriérec, Christophe Di Giorgio, Pierre Vierling,* Antonino Mazzaglia, Norberto Micali, Jacques Defaye* and José M. García Fernández*

β-Cyclodextrin-based polyaminothiourea amphiphiles efficiently condense DNA into nanoparticles (CDplexes); *in vitro* experiments using murine embryo cells showed high transfection rates with very low toxicity profiles.



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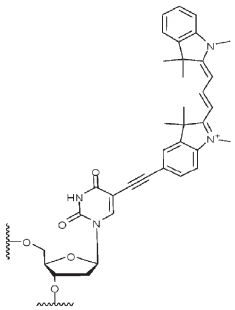
2004

Rigid cyanine dye nucleic acid labels

Adrian Fegan, Pravin S. Shirude and Shankar Balasubramanian*

Cyanine dyes attached to DNA *via* a rigid linker show useful fluorescence and FRET properties without altering the stability of duplex DNA and suggest such constructs may be useful for fluorescence biophysics and assays in nucleic acid systems.

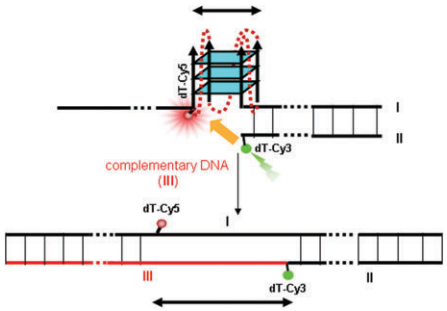


2007

Single molecule conformational analysis of the biologically relevant DNA G-quadruplex in the promoter of the proto-oncogene *c-MYC*

Pravin S. Shirude, Liming Ying and Shankar Balasubramanian*

Single molecule fluorescence spectroscopy has been employed to resolve the conformational heterogeneity, hybridization kinetics and study mutational effects on the *c-MYC* promoter G-quadruplex.

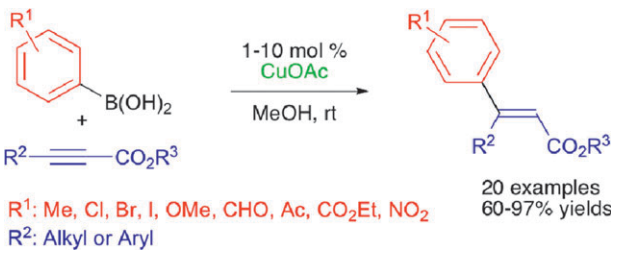


2010

Cu-catalyzed stereoselective conjugate addition of arylboronic acids to alkynoates

Yoshihiko Yamamoto,* Naohiro Kirai and Yu Harada

Cu-catalyzed conjugate additions of arylboronic acids to alkynoates.

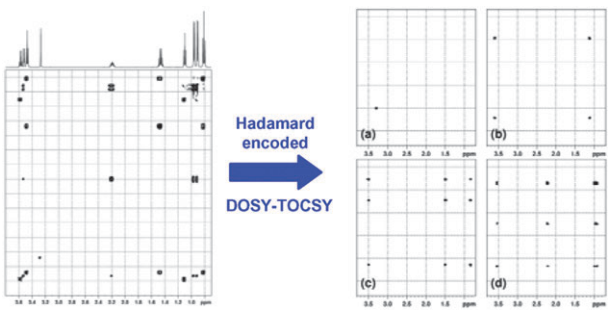


2013

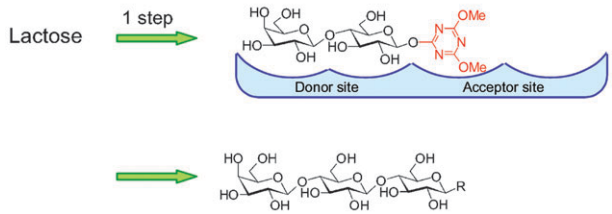
Improved 3D DOSY-TOCSY experiment for mixture analysis

Stéphane Viel* and Stefano Caldarelli

Hadamard encoding allows a 10-fold reduction in minimum experiment time for 3D DOSY homonuclear experiments.



2016

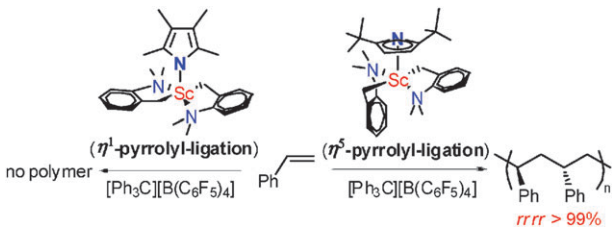


A novel glycosyl donor for chemo-enzymatic oligosaccharide synthesis: 4,6-dimethoxy-1,3,5-triazin-2-yl glycoside

Tomonari Tanaka, Masato Noguchi, Atsushi Kobayashi and Shin-ichiro Shoda*

An efficient glycosyl donor, 4,6-dimethoxy-1,3,5-triazin-2-yl β-lactoside (DMT-β-Lac), which can be prepared directly from lactose in water without using any protecting groups, has been developed for enzymatic glycosylation catalyzed by an endo-1,4-β-glucanase.

2019

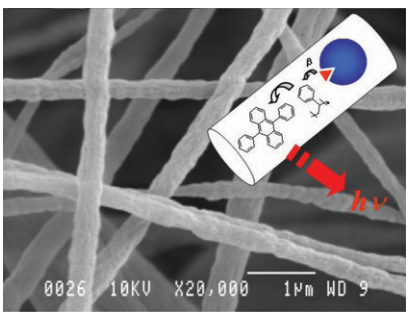


Synthesis and styrene polymerisation catalysis of η^5- and η^1-pyrrolyl-ligated cationic rare earth metal aminobenzyl complexes

Masayoshi Nishiura, Tomohiro Mashiko and Zhaomin Hou*

The cationic rare earth aminobenzyl complexes bearing mono(pyrrolyl) ligands are synthesised and structurally characterised, and the coordination mode of the pyrrolyl ligands is found to show significant influence on styrene polymerisation.

2022

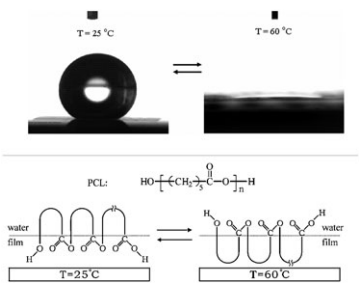


A simple method for preparation of molecularly imprinted nanofiber materials with signal transduction ability

Keiichi Yoshimatsu, Lei Ye,* Patrik Stenlund and Ioannis S. Chronakis*

A simple electrospinning method is developed to introduce signal transduction ability into molecularly imprinted nanofibers, allowing molecular recognition event to be monitored in real time.

2025



New responsive property of poly(ε-caprolactone) as the thermal switch from superhydrophobic to superhydrophilic

Shuxin Hu, Xinyu Cao,* Yanlin Song, Chao Li, Ping Xie and Lei Jiang*

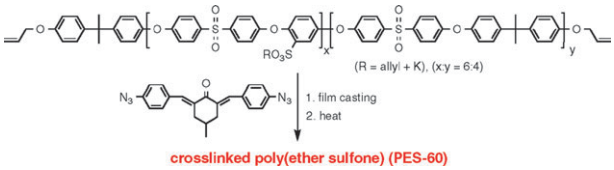
A reversible switch between superhydrophobicity at low temperature and superhydrophilicity at high temperature was fabricated, which resulted from the combination of the different adaptability of the polymer chain upon crystalline/amorphous phase transition and the optimized roughness.

2028

Azide-assisted cross-linked sulfonated poly(ether sulfone)s as stable and highly conductive membranes with low methanol diffusion coefficients

Young-Seok Oh, Hye-Jin Lee, Minji Yoo, Hyoung-Juhn Kim, Jonghee Han, Kyuwon Kim, Jong-Dal Hong and Tae-Hyun Kim*

A novel network structure of the sulfonated poly(ether sulfone)s was prepared by azide-assisted thermal irradiation. The prepared PES-60 membrane offered exceptionally high proton conductivity and a low methanol diffusion coefficient.

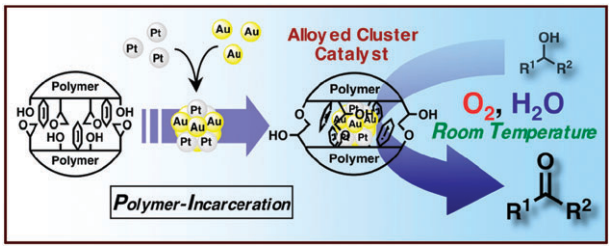


2031

Gold–platinum bimetallic clusters for aerobic oxidation of alcohols under ambient conditions

Hiroyuki Miyamura, Ryosuke Matsubara and Shu Kobayashi*

We have developed gold/platinum alloyed bimetallic cluster catalysts supported on a cross-linked polystyrene derivative, which present much higher activity and selectivity than single metal gold or platinum clusters for aerobic oxidation of alcohols under ambient conditions.

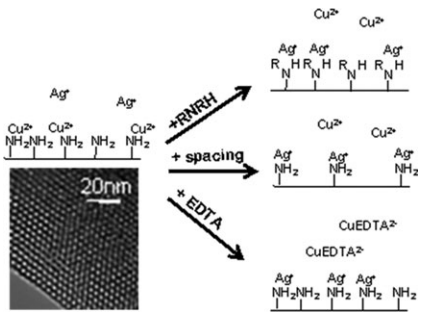


2034

Selective mesoporous adsorbents for Ag^{+}/Cu^{2+} separation

Koon Fung Lam, Xinqing Chen, Chi Mei Fong and King Lun Yeung*

Three different approaches, including (1) manipulating the site chemistry, (2) controlling the spacing between neighbouring sites and (3) altering the adsorbates by the use of chelates, were successfully used to prepare MCM-41 adsorbents with excellent selectivity for silver adsorption from solutions containing copper.

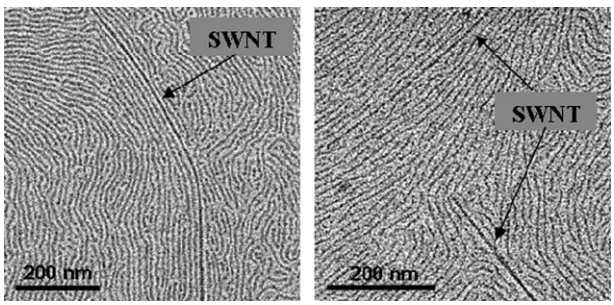


2037

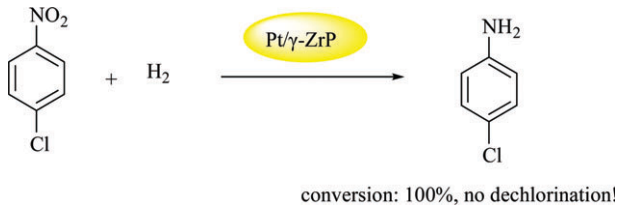
Shear-induced ordering of micellar arrays in the presence of single-walled carbon nanotubes

Einat Nativ-Roth, Oren Regev and Rachel Yerushalmi-Rozen*

Single-walled carbon nanotubes were found to induce elongation and alignment of surfactant micelles in thin films under the action of shear, leading to the formation of ordered micellar arrays over micron lengths.



2040

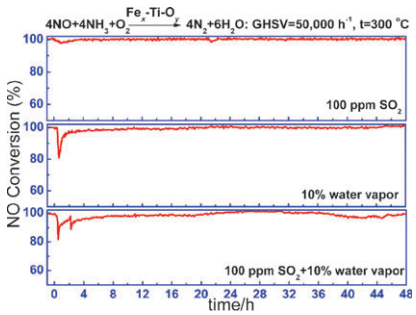


Layered material γ-ZrP supported platinum catalyst for liquid-phase reaction: a highly active and selective catalyst for hydrogenation of the nitro group in *para*-chloronitrobenzene

Fang Wang, Junhua Liu and Xianlun Xu*

Chemoselective hydrogenation of *para*-chloronitrobenzene without any dechlorination over Pt/γ-ZrP catalyst proceeds effectively, which provides a clean and convenient approach to produce useful *para*-chloroaniline with excellent activity and selectivity.

2043



Novel iron titanate catalyst for the selective catalytic reduction of NO with NH_3 in the medium temperature range

Fudong Liu, Hong He* and Changbin Zhang

Novel iron titanate catalyst (Fe_xTiO_y) with a crystallite phase, prepared by a conventional co-precipitation method, showed excellent activity, stability, selectivity and SO_2/H_2O durability in the selective catalytic reduction of NO with NH_3 in the medium temperature range.

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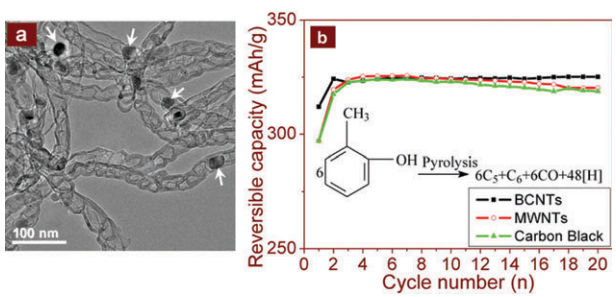
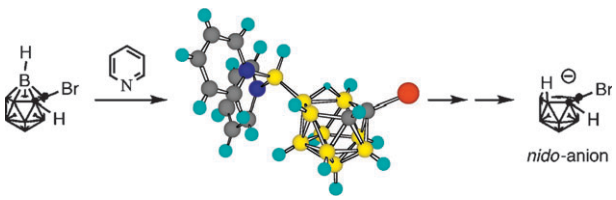


High-yield bamboo-shaped carbon nanotubes from cresol for electrochemical application

Ruitao Lv, Lin Zou, Xuchun Gui, Feiyu Kang,* Yanqiu Zhu, Hongwei Zhu, Jinquan Wei, Jialin Gu, Kunlin Wang and Dehai Wu

Bamboo-shaped carbon nanotubes (BCNTs) were produced by cresol for the first time. The role of cresol in promoting the growth of BCNTs was discussed. Improved electrochemical performances of BCNTs as an anode additive in a lithium ion battery were achieved.

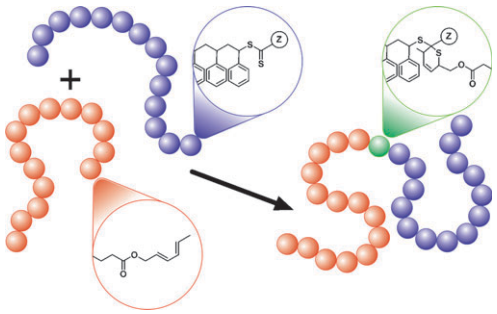
2049

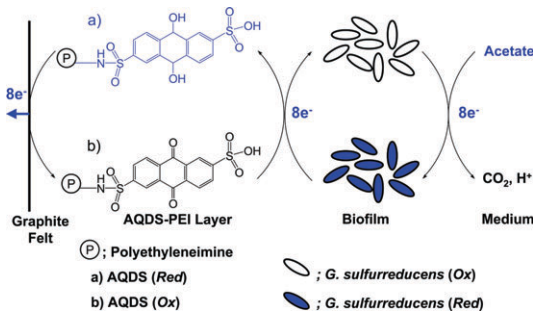


Identification of an intermediate in the deboronation of *ortho*-carborane: an adduct of *ortho*-carborane with two nucleophiles on one boron atom

Yoshiyuki Taoda, Takehiko Sawabe, Yasuyuki Endo,* Kentaro Yamaguchi, Shinya Fujii and Hiroyuki Kagechika*

The 1 : 2 adduct of 1-bromo-*ortho*-carborane and pyridine has been identified as a significant intermediate in the deboronation of *ortho*-carborane to a *nido*-anion.





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Chemical Biology

Chip study confirms protein role in odorant transport

The science of smell

Smells influence much of our behaviour, including what we choose to eat and with whom we flirt; they can also alert us to danger. But, despite its importance, we have never fully understood how we smell. Now, scientists from the French National Research Institute for Agricultural Research (INRA) in Jouy-en-Josas, France, have used lab-on-a-chip technology to shed some light on this complicated process.

Scientists know that aroma molecules, or odorants, bind to olfactory receptors (ORs) which sit under a layer of mucus in the upper section of the nose. There are more than 350 different ORs in humans, and these work in a combinatorial fashion to allow us to smell many more odorants. Odorant binding to an OR sets off a chain of events that converts the chemical binding energy into a neural signal, which we register as a smell.

What is puzzling, though, is how this first binding step works – most odorants are hydrophobic, while the mucus covering the ORs in the nose is aqueous. Scientists have assumed that another species becomes involved to help shuttle the odorant through the mucus layer: an odorant binding protein (OBP). However, an interaction involving all three species had never been demonstrated directly.

Now, Jasmina Vidic, Edith Pajot-Augy and colleagues have observed just such an interaction. Using surface plasmon resonance (SPR) the researchers have studied the binding between the three species on a sensor chip. SPR uses light to excite surface plasmons (electromagnetic waves at a surface). Their oscillation is very sensitive to changes in their environment, and so the binding processes could be monitored on the chip by measuring changes in these oscillations.

JUPITER IMAGES

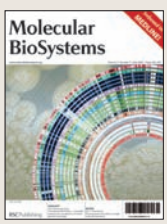
As well as confirming OBP's passive transport role, the French scientists discovered that the protein plays an active role in the nose – preserving OR activity at high odorant concentration. 'There have been some predictions in this direction,' says Vidic, 'however, this feature has never been demonstrated before.'

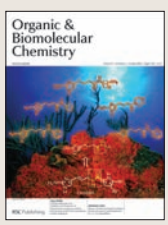
'Label-free detection schemes based on SPR have become increasingly popular for studying many kinds of ligand–receptor interactions,' says Sabine Szunerits, an expert on SPR from the Grenoble Institute of Technology, France. This work, she says, 'shows once more that SPR bioelectronic sensors are powerful tools for investigating biologically pressing questions.'

Freya Mearns

Reference
J Vidic *et al*, *Lab Chip*, 2008, DOI: 10.1039/b717724k

In this issue





Research highlights

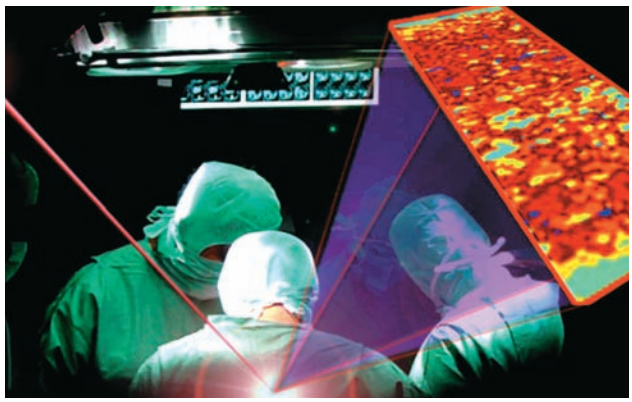
Fast and accurate diagnosis during surgery could save lives

Analysing aneurysms

In the future, doctors may be able to spot life-threatening blood vessel swelling more accurately, thanks to work by French scientists.

Ganesh Sockalingum, from the University of Reims, and co-workers have developed an imaging analysis procedure and used it to investigate infrared images of artery tissue samples. They have improved on current IR tissue imaging, which is already a powerful tool for discriminating between normal and pathological samples in brain, colon or skin cancers. Current methods can often process only one image at a time but the French team's procedure can determine tissue characteristics from several images simultaneously.

Franck Bonnier, a member of the French team, outlines the motivation for the work. During heart surgery, a surgeon can be faced with a dilated aortic wall, he explains. The aorta is the artery that carries oxygenated blood from the heart and if an aortic aneurysm, where the wall is swollen, is not detected in time, the aorta may rupture. This is usually fatal unless treated swiftly. With moderate wall dilation, doctors find it hard to judge whether the aorta needs surgical replacement and there are currently no qualitative tools to guide their decisions.



Imaging analysis could help surgeons to diagnose aneurysms during an operation

Sockalingum's group ensured that its spectroscopic analysis could reliably distinguish healthy and pathological aortic tissues. They then applied colour labelling, which takes only 20 seconds once the images have been obtained, with blue representing healthy tissue and red for damaged tissue. Bonnier says that the images could be used by surgeons who do not have a strong background in spectroscopy and data processing.

Cyril Petibois of the University of Bordeaux, in Talence, France, who works on molecular imaging using IR, says: 'The ability to rapidly give an answer to a surgeon during surgery is the typical role that IR imaging should be able to play in the future.'

Dominique Bertrand, another member of the research team, says that, although the method is still far from practical applications, the know-how developed in the present, complex case could be applied in many fields such as medicine, genetics and biology. *Christina Morrell*

Reference
F Bonnier *et al*, *Analyst*, 2008, DOI: 10.1039/b717164a

Platelets stick together as activators go with the flow

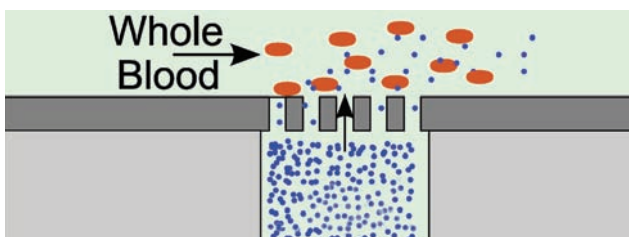
Blood clotting on-chip

Microfluidic technology could help unravel the complex role of clot formation in bleeding disorders.

A microfluidic device, designed by Scott Diamond and Keith Neeves from the University of Pennsylvania in Philadelphia, US, can be used to examine how platelets aggregate into clots when a blood vessel is injured.

The device is unique in that it introduces platelet activators, known to play a critical role in clot formation, at a controlled rate into bloodflow outside the body. 'Our group is interested in developing technologies that mimic features of in vivo blood vessels using flow-based in vitro systems,' says Diamond.

The set-up is based on a three-layer system: a top channel containing blood flowing under physiological conditions, a perpendicular channel containing activator solution, and a polycarbonate membrane between. A controlled amount of activator can be released into the blood through gaps in the membrane. The researchers can then dismantle the device after different experiments to examine how the conditions affect platelet aggregation on the membrane.



Platelet activators (blue) mix with blood flowing through a microfluidic device leading to clots on the membrane between

Diamond explains that, by helping scientists to understand platelet aggregation, the device could be of use for medical research. 'The mechanisms that contribute to clot stability or instability would be useful information in identifying therapeutic strategies for genetic blood disorders, such as haemophilia,' he says. 'Another potential application is flow-based drug screening of anti-platelet therapies to prevent heart attacks.'

Diamond adds that a future challenge will be proving these techniques can yield results that are as good as or better than animal models for predicting how well such new therapies will work. 'In vascular injury, for example, there is a complex interplay between the extracellular matrix, platelets and cells. Currently, no in vitro system can probe all of these interactions,' he admits. 'However, advances in microfluidic techniques allow a very large parameter space to be explored in a combinatorial manner with minimal volumes of reagents and tissue.' *Stephen Wilkes*

Reference
K B Neeves and S L Diamond, *Lab Chip*, 2008, DOI: 10.1039/b717824g

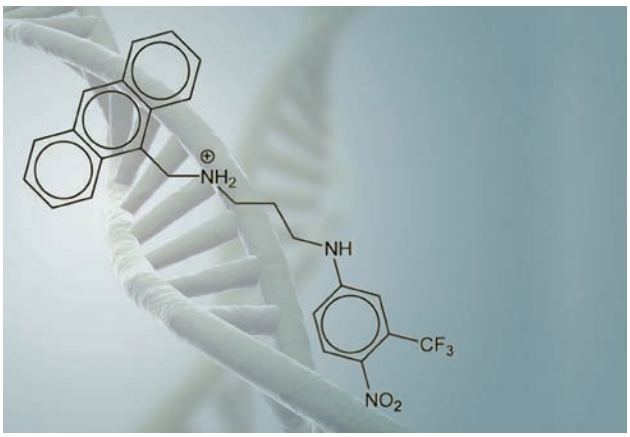
Tumour treatments see the light

DNA-seeking probes could deliver anticancer agents right to the heart of tumour cells, say chemists in Italy.

Nitric oxide (NO) is a promising anticancer agent, killing cancer cells mainly by reacting with their DNA, causing the strands to break. To deliver NO directly to DNA, Salvatore Sortino and Fiorella Callari from the University of Catania have combined a light-triggered NO donor with a DNA binding agent.

Sortino had previously developed a nitroaniline-based system, which releases NO when irradiated with visible light. To develop the new NO delivery probe, Sortino attached the nitroaniline derivative to anthracene, a flat aromatic structure known to nestle tightly into the grooves in the DNA double helix. Sortino then showed that the bifunctional system did bind to DNA, and successfully released NO when triggered by light.

'The next step is to find suitable delivery vehicles to carry the NO donor into the cell compartments, and to evaluate its ability to induce DNA photorupture and phototriggered cell death,' Sortino says. But the potential applications of triggered NO release are not limited to cancer therapy, he adds.



Attaching an anthracene group to an NO donor creates a DNA-binding NO delivery system

Reference
F L Callari and S Sortino, *Chem. Commun.*, 2008, 1971 (DOI: 10.1039/b800132d)

Gjumrakch Aliev, who studies the role of NO in biology at the University of Texas at San Antonio, US, agrees that controllable methods for NO release will have wide-ranging applications, including in the clinic. 'NO is a small molecule, able to cross the blood–brain barrier, so it has the potential to treat neurological disorders,' he adds.

James Mitchell Crow

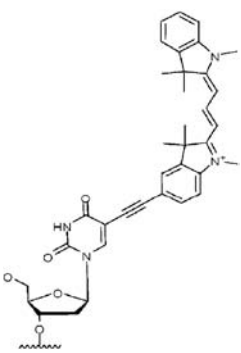
The rigid future of DNA labels

Chemists have linked fluorescent tags to DNA to minimise unwanted interactions with the double helix.

Cyanine dyes are often used as fluorescent labels for DNA, proteins and other biomolecules. Shankar Balasubramanian and colleagues at the University of Cambridge, UK, attached these dyes to DNA by a rigid linker.

Widely-used methods to attach cyanine dyes to DNA employ a flexible linker instead, explains Balasubramanian. 'We and others have shown that this results in a dye–DNA interaction that alters the stability of the DNA double helix.' In contrast, the UK team found that using an ethynyl linker fixed the dye's geometry and position, preventing it from interacting with the DNA helix and so changing its stability and structure.

'It is an enduring challenge to develop tags that accurately report on – without perturbing – biomolecule structure and/or function,' says Bruce Armitage from Carnegie Mellon University, in Pittsburgh, US, who works in the field of biomolecule recognition. 'This linker elegantly achieves this elusive goal.'



Linking a cyanine dye to DNA with a rigid linker reduces its interactions with the double helix

Reference
A Fegan, P S Shirude and S Balasubramanian, *Chem. Commun.*, 2008, 2004 (DOI: 10.1039/b801629a)

'There is considerable interest in labelling DNA and RNA with fluorescent dyes for applications that include fluorescence biophysics, genetic analysis, gene sequencing and nanoscience,' says Balasubramanian, explaining his motivation for the work.

Duncan Graham, a DNA researcher from the University of Strathclyde, in Glasgow, UK, agrees that the new method has potential for biological science. 'This work has implications in many areas of bioanalysis,' he says. *Sarah Corcoran*

News in brief

Spiky sponges share their secrets
Enzymes that make sponges spiky are promising leads for silicon-based materials, say UK scientists.

Growing cells in patterns
Using a simple stamping method, US chemists are creating cell patterns on ordinary microscope coverslips.

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Arsenic exposure from rice milk
Researchers have found that levels of arsenic in rice milk exceed EU and US drinking water standards.

Cleaning up after nerve agents
US scientists have demonstrated that cheap, easily prepared chemicals can break down organophosphate nerve agents to non-hazardous materials.

In the beginning...
In this month's interview, Kenso Soai discusses the origin of chirality in life.

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This month in *Chemical Technology*

Cellular power plants fuel molecular motors
Mitochondria have been used to power miniature motors for microfluidic devices.

Nerve agent detector on a chip
A microfluidic device that can identify exposure to sarin could help identify individuals needing treatment at sites of terrorist attack.

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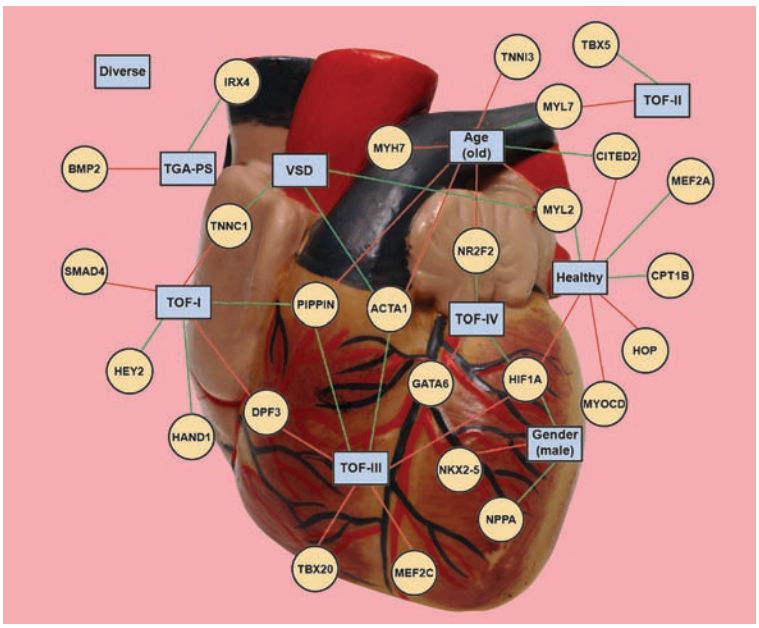
Linking changes in gene expression to heart disease

The heart of the matter



Data analysis leads to networks showing relationships between gene expression and characteristics related to heart disease

German scientists are unravelling the genetic basis of diseases by combining computational biology techniques.

Silke Sperling of the Max Planck Institute for Molecular Genetics, Berlin, and colleagues have used various data analysis methods to study gene expression. By looking at how gene expression levels vary between heart patients with different symptom patterns they were able to identify genes that may be involved in certain heart conditions. 'We are very excited,' says an enthusiastic Sperling. 'It is nice to puzzle things together and see meaningful data come out.'

With their data the researchers drew up networks showing how the products of some genes regulated the expression of others. The method can predict interactions between transcription factors – proteins that regulate gene expression – and their targets, which is a key feature, explains Sperling.

Sperling's research confirmed earlier results achieved by in vitro biochemical methods, proving the reliability of the approach. But not only that, the group also found new interactions between transcription factors and targets, showing that the method can be used to explore the genetic processes underlying disease.

The researchers say that the key behind their approach's success is in how the computational techniques are combined, producing more significant and reliable results than using individual methods alone.

The research is at the centre of Sperling's interest in the genetics of heart disease, but she says it could benefit studies into any medical condition. The method is also capable of handling large amounts of data, Sperling adds. 'It was important to prove the method first. Next we will try to go to the genome-wide level.'

Danièle Gibney

Reference
M Toenjes *et al*, *Mol. BioSyst.*, 2008, DOI: 10.1039/b800207j

In the current issue of Research Articles...

Digital microfluidics for cell-based assays
Irena Barbulovic-Nad *et al*, *Lab Chip*, 2008, **8**, 519 (DOI: 10.1039/b717759c)

Chemical labels and natural element tags for the quantitative analysis of bio-molecules
Andreas Prange and Daniel Pröfrock, *J. Anal. At. Spectrom.*, 2008, **23**, 432 (DOI: 10.1039/b717916m)

Mixed valent sites in biological electron transfer
Edward I Solomon *et al*, *Chem. Soc. Rev.*, 2008, **37**, 623 (DOI: 10.1039/b714577m)

Sub-micromolar affinity of *Escherichia coli* NikR for Ni(II)
Rutger E M Diederix *et al*, *Chem. Commun.*, 2008, 1813 (DOI: 10.1039/b719676h)

Detection of nitric oxide in single cells
Xiaoying Ye *et al*, *Analyst*, 2008, **133**, 423 (DOI: 10.1039/b716174c)

Gene regulation technologies in zebrafish
Hanife Esengil and James K Chen, *Mol. BioSyst.*, 2008, **4**, 300 (DOI: 10.1039/b718447f)

Yatakemycin: total synthesis, DNA alkylation, and biological properties
Mark S Tichenor and Dale L Boger, *Nat. Prod. Rep.*, 2008, **25**, 220 (DOI: 10.1039/b705665f)

Diversity-oriented synthesis; a spectrum of approaches and results
Richard J Spandl *et al*, *Org. Biomol. Chem.*, 2008, **6**, 1149 (DOI: 10.1039/b719372f)

CCD imaging of basal bioluminescence in larval fireflies: clues on the anatomic origin and evolution of bioluminescence
V R Viviani *et al*, *Org. Biomol. Chem.*, 2008, **7**, 448 (DOI: 10.1039/b718016k)

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Interview

Managing chaos

Hagan Bayley talks to Laura Howes about the constraints of defining science and what he's learnt from the business world

Hagan Bayley

Hagan Bayley is professor of chemical biology at the University of Oxford, UK. His research interests include the molecular engineering of membrane proteins for applications in basic science and biotechnology. Hagan is a *Molecular BioSystems* editorial board member.

Why did you decide to be a scientist?
I think it was as simple as enjoying science and mathematics at school. Becoming a scientist just happened rather than being planned.

You did your undergraduate degree in Oxford. Has the course altered much since then?
The subject matter is frighteningly unchanged. I think what Oxford is trying to do is turn out students who really know *chemistry*, which is different to the multidisciplinary approach at other universities. You can argue that the lack of change is good, that in the three years as an undergraduate you have to learn the basis for everything that comes later. But you can also argue that it's a little out of touch with what's going on, not in the chemical sciences but in science in general.

After your degree you moved to the United States. Do you prefer it over there?
I was in the US from 1974–2003 so my whole career was in the States before I came back to Oxford. I've never stayed in one place for more than about eight years and I've really enjoyed every place I've lived. I can't say I preferred the States. Oxford is hugely international; there's an enormous amount going on here and it's close to London without having to live in London. There's a lot going on in life. You have to find your top 10 per cent and enjoy it.

How do you define chemical biology?
I prefer not to define chemical biology. I think chemistry, biology and physics are words people have used to put boundaries around things that don't really exist. I think terms like chemical biology are probably useful for dealing with the administration in a university or raising money from a research council, but scientifically they can be quite constraining. We don't need people to tell us who we are or what to do. We need freedom to operate if we are going to do new science.

Do you think collaborations are the way forward or do you prefer knowing exactly what goes on in your lab?
I like local control but I believe in chaos too. The few new things that you do in your lifetime come from having the freedom to experiment. We're not a factory turning out a product; we bring good people together and see what emerges.

It's very useful to have all the components of a project in your own lab so you can easily have a chat and sort things out. I've tried to bring a lot of technologies into the lab and I wouldn't pretend to be an expert in any one of them but bringing them together is amazingly powerful. So in some ways, you're a bit more like an architect – you bring people with different skills together to come up with a beautiful and functional building. But obviously, to extend the analogy, to plan a city would require collaboration between groups. Some people like to collaborate and others like to bring people together and watch it unfold in front of their eyes, which is more my style.

You have a spinout company, Oxford NanoLabs. How is it going?
Pretty well! We started with stochastic sensing, an area that had matured in the lab, and we set up a company to do it. As it happens, we are now focusing on single molecule DNA sequencing, which is a very exciting area, so it's frontline science as well.

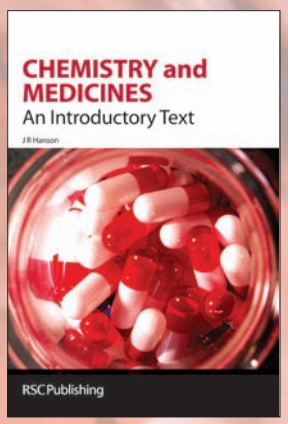
As an academic, it has been really interesting being able to turn much more fire power onto a problem and see how quickly something can move forward in a business. Working with business people has been very interesting as well. I do think you need a certain amount of chaos to generate new ideas and discover new things in your lab but you need management as well, which I'm learning at a late stage from these guys.

Apart from science, what fascinates you?
Architecture fascinates me. Nowadays, it's a mixture of engineering and the arts. I'm very interested in the design of objects for human use. Everything from tools and vehicles to buildings should both work and look beautiful, a challenge that is often unmet.

Chemistry and Medicines

An Introductory Text

By J R Hanson



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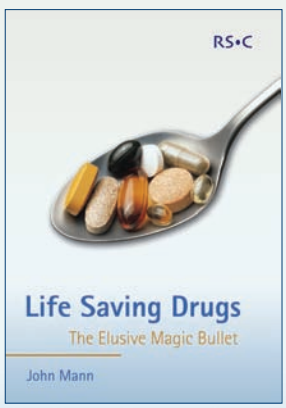

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Instant insight

Crossing the cell membrane

Shana Kelley of the University of Toronto in Canada reveals how cell-penetrating peptides deliver the goods when it comes to biology and medicine

A universal platform to deliver bioactive agents into cells is an attractive goal for myriad applications. Although several useful drug delivery vectors have emerged in recent years, including liposomes, viral vectors, dendrimers, and polymer-based nanoparticles, each has been limited by some feature: difficult synthetic procedures, toxicity, low stability, or a restricted cargo range. The ideal cellular transporter would be low cost, non-toxic, and could transport any cargo across the cellular membrane. Such a transporter would be of enormous value to deliver drugs, imaging agents, and biomolecules such as proteins and DNA – but could such a versatile transporter exist?

The discovery of a cell-permeable class of molecules in the 1990s aroused immediate interest. The finding that simple biomolecules – small synthetically-accessible peptides – could traverse the cell membrane hinted that a versatile transporter could finally be on the horizon. Since this first discovery, research on these cell-penetrating peptides (CPPs) has been conducted at the interface of the chemical, biological, and medical communities with important contributions from each of these disciplines. Hundreds of studies have been completed, uncovering important aspects of CPPs' chemical features, interactions with membranes, how they enter into cells, and their scope as delivery vectors.

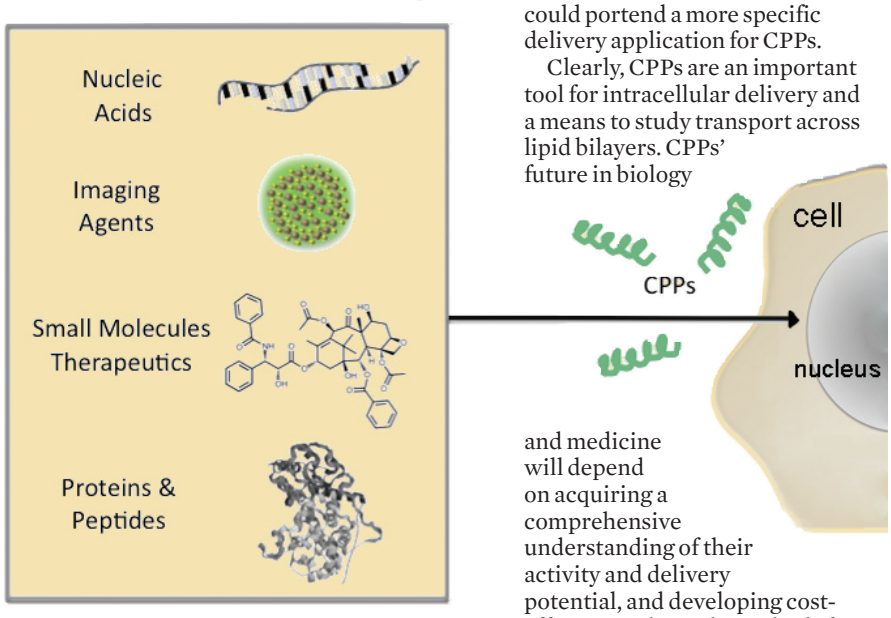
Shortly after the first CPPs – penetratin from *Drosophila melanogaster* and Tat from HIV – were discovered, several more cell-penetrating sequences were identified from natural sources. This was closely followed by the development of synthetic sequences incorporating features of natural CPPs found to be critical for uptake into cells, specifically, positive charge and guanidinium headgroups. Not only were peptide sequences developed using the principles learned from natural CPPs, but other chemical scaffolds were also adapted to have cell-penetrating capacity, including beta-peptides, carbamates, and dendrimers. Studies elucidating the CPP counterion role in crossing the lipid bilayer were also critical in providing insight into the chemical modifications that would mediate cellular uptake.

What is perhaps most exciting about CPPs is the wide variety of cargoes that these short peptide sequences can deliver by mediating their uptake across the cell membrane. Using both covalent and non-covalent linkages, CPPs have transported macromolecules such as proteins, antibodies, and nucleic acids, therapeutics ranging in size and chemical character, and imaging agents, including quantum dots and magnetic particles – CPPs' potential as a universal delivery agent is evident. Moreover, their ability to preserve biological activity for therapeutic cargoes makes the CPP delivery approach truly practical.

An intriguing future direction for CPPs is the potential to achieve targeted delivery into specific organelles within cells. Imaging studies using fluorophore-labelled CPPs have shown that they locate predominantly in the nucleus and cytoplasm, but recent studies have shown that short, synthetic, cell-permeable peptide sequences can be engineered to locate within mitochondria. Critical chemical parameters modulate this localisation. Given mitochondria have roles in many cellular processes and their connection with the treatment of neurodegenerative diseases and cancer, this finding could portend a more specific delivery application for CPPs.

Clearly, CPPs are an important tool for intracellular delivery and a means to study transport across lipid bilayers. CPPs' future in biology and medicine will depend on acquiring a comprehensive understanding of their activity and delivery potential, and developing cost-effective and simple methods for their application.

Read Kelley et al*'s perspective 'Cell-Penetrating Peptides as Delivery Vehicles for Biology and Medicine' in a forthcoming issue of* Organic and Biomolecular Chemistry.

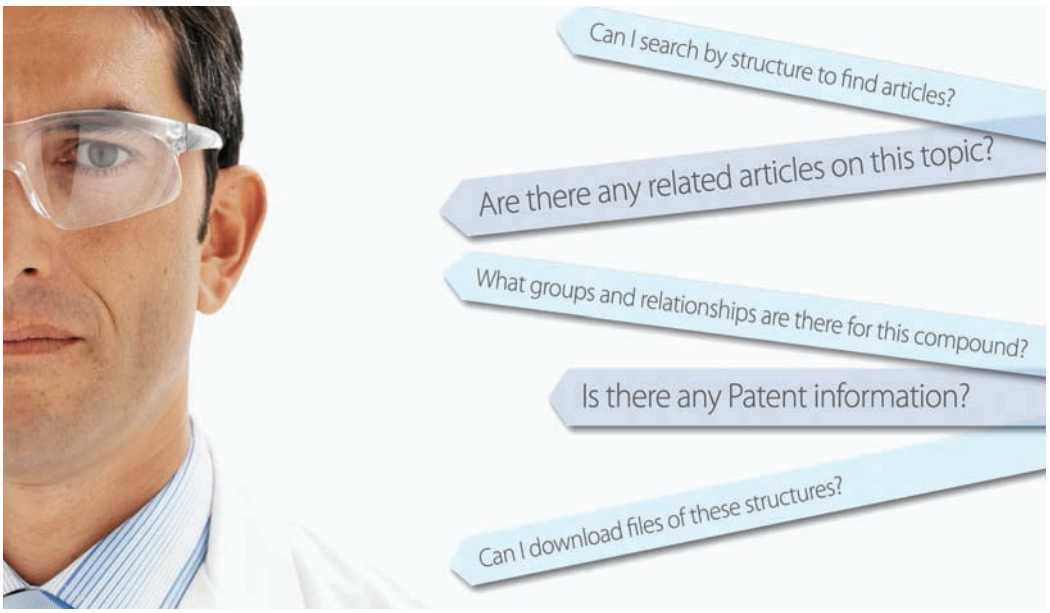


Cell-penetrating peptides can carry many different cargoes into a cell

Reference
K M Stewart, K L Horton and S O Kelley, *Org. Biomol. Chem.*, 2008, DOI: 10.1039/b719950c

Essential elements

Faced with questions?



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