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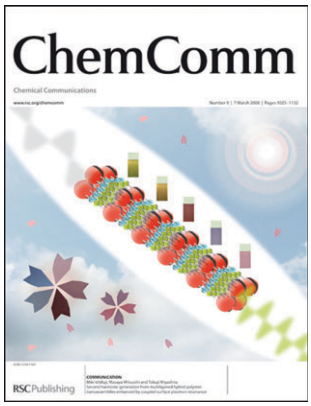
ISSN 1359–7345 CODEN CHCOFS (9) 1025–1132 (2008)

Cover
See Simon R. Hall *et al.*, page 1055.
Supercuttle! Cuttlebone has been used as a biotemplate in the synthesis of the first high-temperature superconductor with a regular macroporous morphology. 'Cuttlefish image by Todd Stailey - Tennessee Aquarium'. Image reproduced by permission of Emily Campbell, Stuart C. Wimbush and Simon R. Hall from *Chem. Commun.*, 2008, 1055.



Inside cover
See Masaya Mitsuishi *et al.*, page 1058.
Multilayered hybrid polymer nanoassemblies with polymer nanosheets and gold nanoparticles show beautiful colors and effective second harmonic light enhancement. Image reproduced by permission of Miki Ishifuji, Masaya Mitsuishi and Tokuji Miyashita from *Chem. Commun.*, 2008, 1058.

CHEMICAL BIOLOGY

B17

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
March 2008/Volume 3/Issue 3
www.rsc.org/chembiology

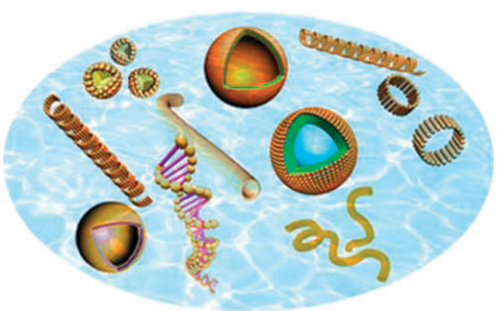
FEATURE ARTICLE

1043

Aqueous self-assembly of aromatic rod building blocks

Ja-Hyoung Ryu, Dong-Je Hong and Myongsoo Lee*

Rod amphiphiles consisting of aromatic rigid segments and hydrophilic flexible chains can self-assemble into a variety of supramolecular structures including capsules, tubules and helical nanofibers in aqueous solution.



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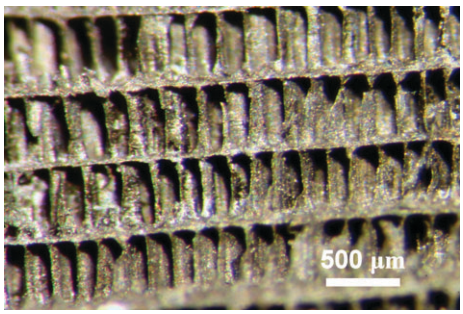

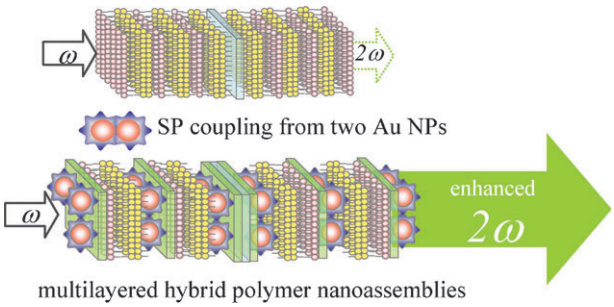

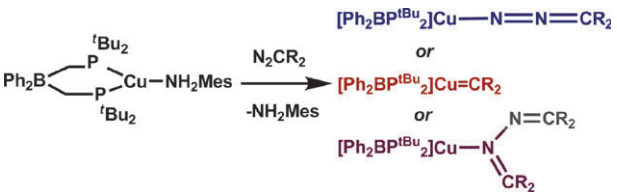

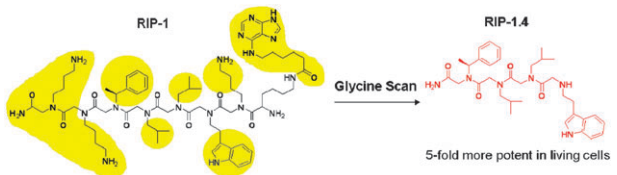

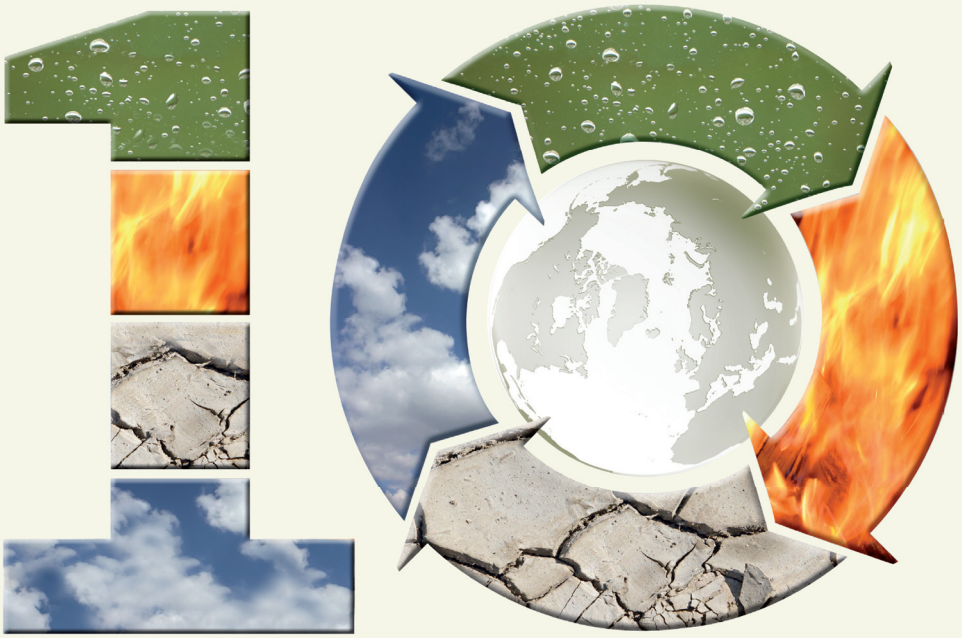

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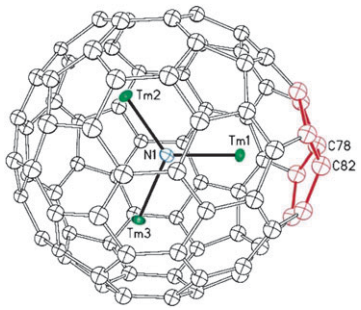

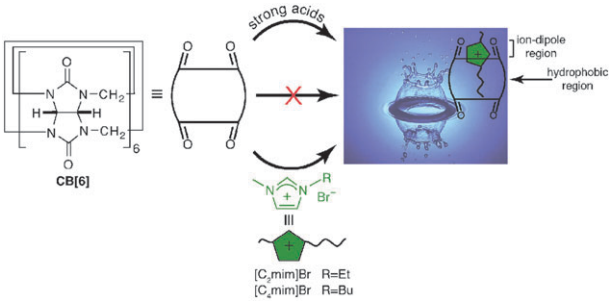

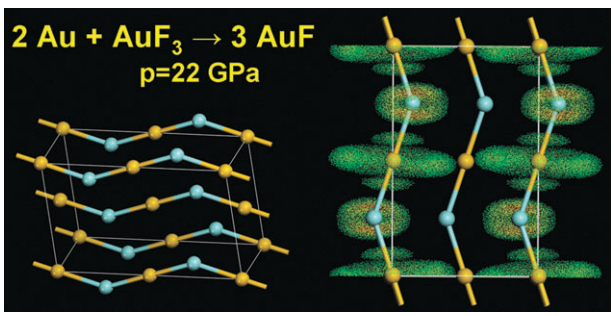

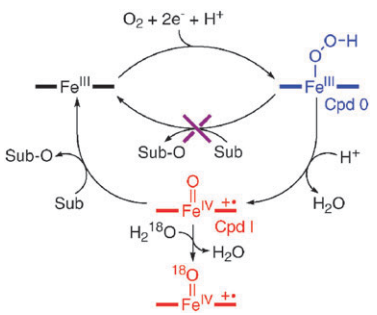

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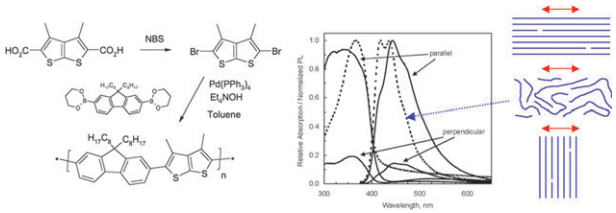
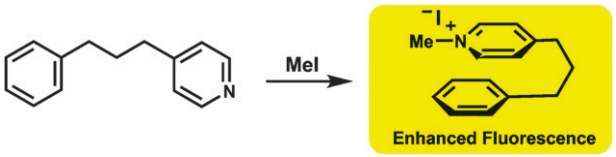


An alignable fluorene thienothiophene copolymer with deep-blue electroluminescent emission at 410 nm

Malte C. Gather, Martin Heeney, Weimin Zhang, Katherine S. Whitehead, Donal D. C. Bradley, Iain McCulloch and Alasdair J. Campbell*

An alignable, liquid-crystalline fluorene fused-ring thienothiophene copolymer has been synthesized with electroluminescence peaking at 410 nm for deep blue, polarised emission in polymer light-emitting diodes, light-emitting transistors and photonic structures.

1082

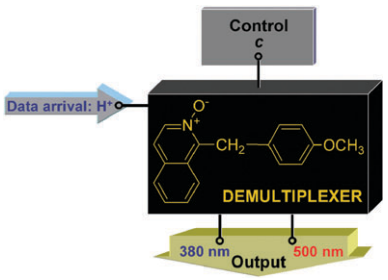


Intramolecular cation–π interactions control the conformation of nonrestricted (phenylalkyl)pyridines

Isabella Richter, Jusaku Minari, Philip Axe, John P. Lowe, Tony D. James, Kazuo Sakurai, Steven D. Bull* and John S. Fossey*

NOEsy and fluorescence spectroscopy reveal that conversion of conformationally flexible (phenylalkyl)pyridines into their corresponding *N*-methyl-pyridinium iodides results in intramolecular π-stacking.

1085

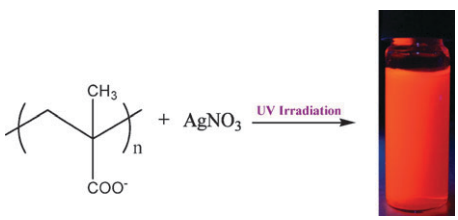


A molecular 1 : 2 demultiplexer

Ezequiel Perez-Inestrosa,* Jose-María Montenegro, Daniel Collado and Rafael Suau

A dual-channel fluorescent molecule runs as a 1 : 2 digital demultiplexer which can drive a single signal (proton) to two different destinations as a fluorescent photonic response.

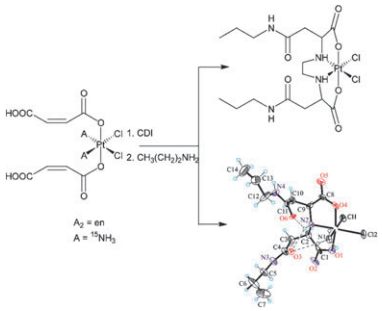
1088

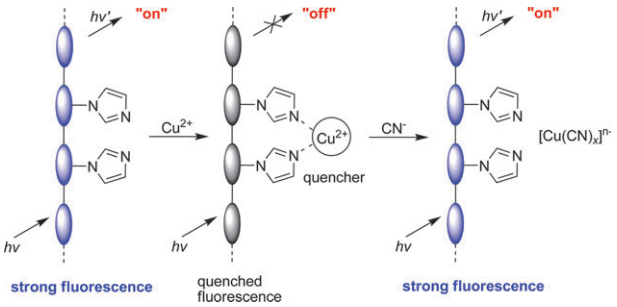


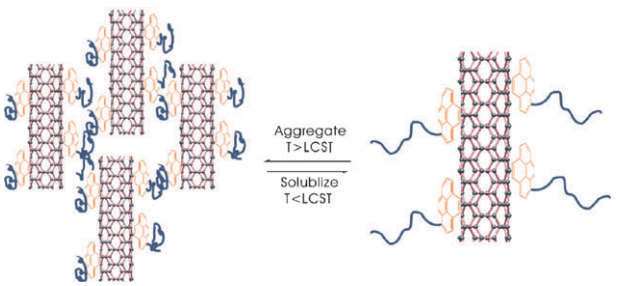
Facile preparation of water-soluble fluorescent silver nanoclusters using a polyelectrolyte template

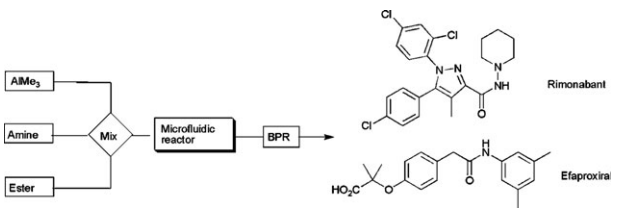
Li Shang and Shaojun Dong*

We report a new approach for the synthesis of fluorescent and water-soluble Ag nanoclusters, using the common polyelectrolyte poly(methacrylic acid) as the template.









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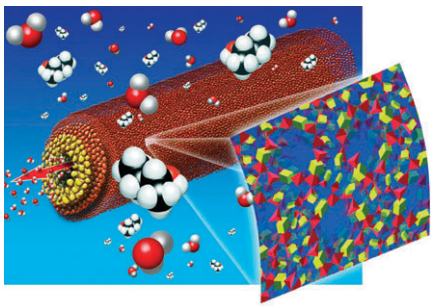
1103

Hybrid ceramic nanosieves: stabilizing nanopores with organic links

Hessel L. Castricum,* Ashima Sah, Robert Kreiter, Dave H. A. Blank, Jaap F. Vente and Johan E. ten Elshof*

A highly hydrothermally stable hybrid molecular sieving membrane was synthesized using bis(triethoxysilyl)ethane. Mechanically supported by porous alumina, the organically bridged ceramic membrane remains highly selective for years.

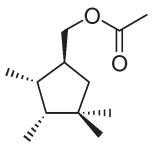


1106

Determination of the absolute configuration of the sex pheromone of the obscure mealybug by vibrational circular dichroism analysis

Bruno Figadère, Frank J. Devlin, Jocelyn G. Millar and Philip J. Stephens

Absolute configurations of the kinetically resolved enantiomers of pheromone **1** were determined by matching the experimentally measured spectrum of (+)-**1** with that calculated from density-functional theory.



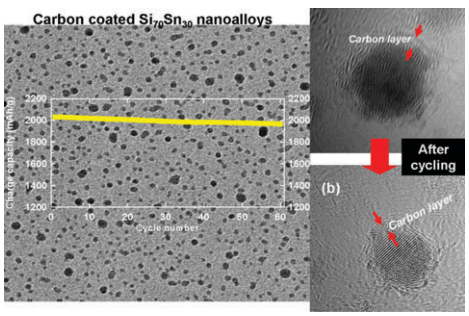
(+)-(1*S*,2*S*,3*R*)-1

1109

High capacity carbon-coated $Si_{70}Sn_{30}$ nanoalloys for lithium battery anode material

YooJeong Kwon and Jaephil Cho*

Carbon-coated $Si_{70}Sn_{30}$ nanoalloys with a particle size <10 nm were prepared from butyl-capped analogues *via* firing at 900 °C under a vacuum and showed a reversible capacity of 2032 mAh g^{-1} and excellent capacity retention.

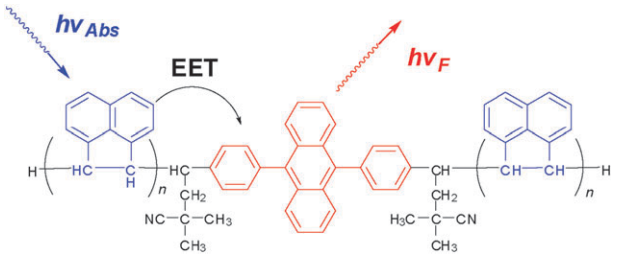


1112

Controlled synthesis of luminescent polymers using a bis-dithiobenzoate RAFT agent

Ming Chen, Kenneth P. Ghiggino,* Ezio Rizzardo, San H. Thang and Gerard J. Wilson

A higher efficiency of excitation energy transfer occurs to a luminescent diphenylanthracenyl acceptor incorporated at the centre, rather than the end, of an acenaphthylene polymer chain.



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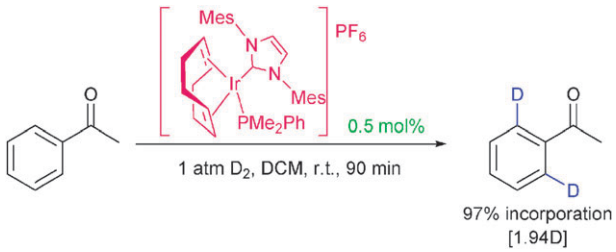
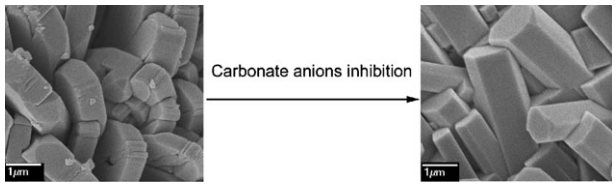


Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

Jack A. Brown, Stephanie Irvine, Alan R. Kennedy, William J. Kerr,* Shalini Andersson and Göran N. Nilsson

Practically convenient methods have been developed for the preparation of new iridium complexes, possessing bulky *N*-heterocyclic carbene and phosphine ligands; these routinely handled complexes are highly active catalysts within directed hydrogen isotope exchange processes.

1118

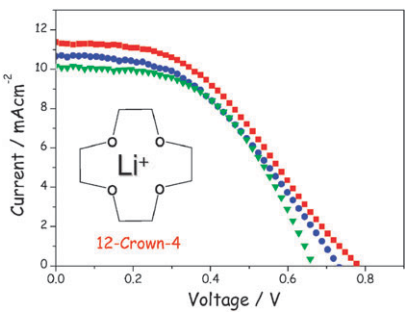


Carbonate anions controlled morphological evolution of $LiMnPO_4$ crystals

Haisheng Fang, Liping Li, Yong Yang, Guofeng Yan and Guangshe Li*

Two-dimensional and one-dimensional crystals of $LiMnPO_4$ were synthesized *via* a hydrothermal method without using any template. The carbonate anions inhibition was considered to be the reason for the formation of one-dimensional $LiMnPO_4$ crystals.

1121

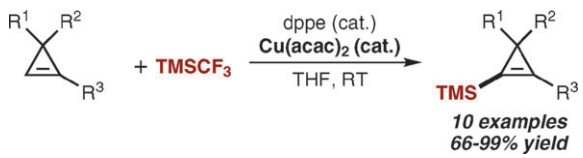


Enhancement of photocurrent generation and open circuit voltage in dye-sensitized solar cells using Li^+ trapping species in the gel electrolyte

João Eduardo Benedetti, Marco Aurelio de Paoli and Ana Flávia Nogueira

The addition of 12-crown-4 ether in a gel polymer electrolyte based on a PEO copolymer increases both the photocurrent and open-circuit voltage values in DSSC. This effect is due to the trapping of Li^+ ions present in the electrolyte.

1124



Copper-catalyzed silylation of cyclopropenes using (trifluoromethyl)trimethylsilane

Euan A. F. Fordyce, Yi Wang, Thomas Luebbers and Hon Wai Lam*

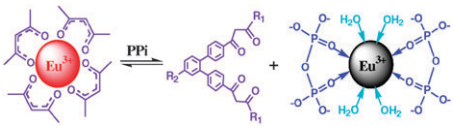
A variety of cyclopropenes undergo direct silylation using (trifluoromethyl)trimethylsilane in the presence of a copper–bisphosphine catalyst. Under these conditions, cyclopropenes that might otherwise undergo ring-opening are silylated efficiently.

1127

Europium(III) complex-based luminescent sensing probes for multi-phosphate anions: modulating selectivity by ligand choice

Na Shao, Jianyu Jin, Guilan Wang, Ying Zhang, Ronghua Yang* and Jingli Yuan*

Four tetradentate β-diketonate–Eu^{3+} complexes were developed as probes for the luminescent sensing of multi-phosphates. By using an appropriate ligand, the pyrophosphate ion (PPi) could be selectively and sensitively detected.



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Chemical Biology

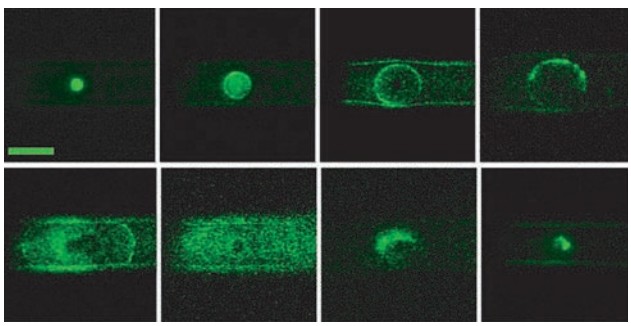
Cells spill their contents as the bubble bursts for on-chip analysis

Laser beam hits tiny target

Chemists looking to analyse single cells have combined lab-on-a-chip techniques with lasers to quickly and accurately burst the cells open.

Vasan Venugopalan, at the University of California, Irvine, US, and colleagues used pulsed laser microbeams to burst the individual cells in a microfluidic device. The ability to rapidly open (lyse) a cell to examine its content is important when analysing biochemicals such as signalling and messenger molecules, since these can break down within seconds, said Venugopalan. It is also important to achieve high sample throughput.

Venugopalan fine-tuned the lysis process by loading sample cells with fluorescent dyes, and using a rapid camera to capture what happens in the nanoseconds after the cell is hit by the laser pulse. A pulse focused within a few micrometres of the cell produced a rapidly expanding bubble which broke the cell membrane. The growing bubble's excess energy was absorbed as the walls of the microchannel deformed outwards. But as the bubble then collapsed and the walls snapped back into place, the cell contents were re-localised into an area barely any bigger than the original cell, said Venugopalan, which should aid subsequent analysis.



A cell bursts inside a microfluidic channel, deforming the walls; as the walls snap back, the cell contents re-localise

Venugopalan pointed out that using laser irradiation to burst the cell requires no specialised on-chip instruments – unlike previous electrical methods which need on-chip electrodes. 'This can simplify device design, and provides the flexibility to accomplish cell lysis at different locations on the chip.'

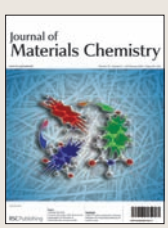
Andrew deMello, who develops microfluidic systems at Imperial College London, UK, said the work was very timely, given the current interest in analysing single cells on-chip. 'The process is highly controllable, and allows you to do the analysis of the released cell content there and then,' he said. 'Pulse lasers are now routinely available, out of a catalogue, and theoretically you could integrate the laser with your normal optical detection equipment.'

Venugopalan now plans to start using the device in cell analysis. 'We are pursuing multiple applications, primarily for biochemical analysis of cell lysates, as well as understanding the cellular response to laser-induced perturbations,' he said.

James Mitchell Crow

Reference
P A Quinto-Su *et al*, *Lab Chip*, 2008, DOI: 10.1039/b715708h

In this issue



Research highlights

Ligands recognise DNA structures implicated in cancer cell immortality

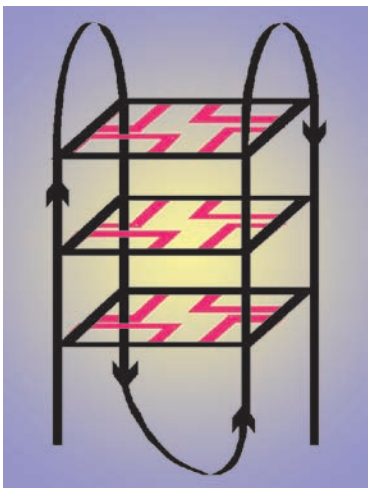
Discriminating ligands select square DNA

Ligands specific for cancer-linked DNA structures are among a series of compounds that could help scientists trying to understand why DNA folds into squares.

G-quadruplexes occur naturally in nucleic acids, and are formed as four guanine residues assemble in a planar arrangement. Now, a group led by Shankar Balasubramanian at the University of Cambridge, UK, has synthesised ligands that bind to these structures selectively.

Balasubramanian's group used a class of compounds called triarylpyridenes as the template for designing its ligands, and varied the aromatic groups attached to the central pyridine structure. The compounds' interactions with different DNA structures were studied and some compounds were found to show selectivity for a G-quadruplex in a telomere – a repeat sequence at the end of a DNA strand.

Telomeric G-quadruplexes are involved in cell replication and death and often implicated in cancer cells' immortality. They are potential anticancer targets, and ligands that interfere with telomere maintenance are the subject of much research.



G-quadruplexes are formed when four guanine residues assemble into a square

Reference
Z A E Waller *et al, Chem. Commun.*, 2008, DOI: 10.1039/b718854d

Jörg Hartig from the University of Konstanz, Germany, who works on using quadruplexes to regulate nucleic acid function, is impressed with the work and the specificities for distinct quadruplex sequences. 'In addition to their potential in cancer therapy, the triarylpyridenes could enable researchers to specifically address one quadruplex structure while leaving other G-rich sequences unaffected,' he said.

'Molecules that bind selectively to these DNA motifs will help us understand G-quadruplex function in cells,' explained Balasubramanian. He added that the group will now evaluate its compounds to determine how they affect cellular processes.

Balasubramanian suggested that there may be thousands of G-quadruplex forming motifs in cells, all ever so slightly different. Looking to the future, the chemists see their challenge in designing molecules that discriminate between the quadruplexes well enough to allow the function of each quadruplex to be investigated individually.

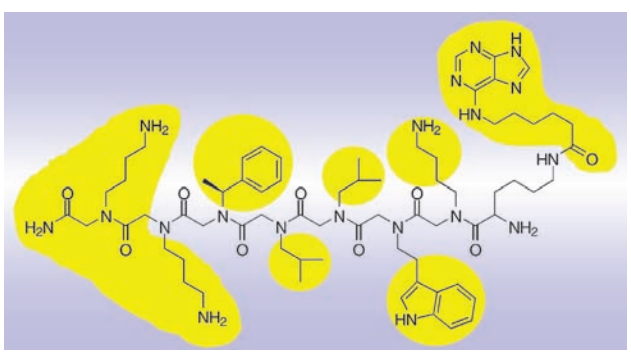
Laura Howes

Side-chain stripping leads quickly to a smaller, more potent proteasome inhibitor

Drugs cut back to their bare essentials

Removing unnecessary atoms from compounds uncovered in preliminary drug screens could simplify the drug development process, say US researchers. With this in mind the American team has developed a method to identify the biologically active sections of these pharmaceutical leads.

The decreasing number of new drugs emerging from pharmaceutical pipelines is challenging medicinal chemists to cultivate fresh approaches to drug design and development. In response to this, Thomas Kodadek and co-workers at the University of Texas Southwestern Medical Center, in Dallas, developed their approach to identify the smallest active fragment – the minimal pharmacophore – of peptoid compounds. Peptoids are similar to peptides but with the side-chain connected to the nitrogen atom rather than the adjacent α-carbon.



Deleting side-chains (yellow) one-by-one from a proteasome inhibitor identifies which are crucial and which not

Reference
H-S Lim *et al, Chem. Commun.*, 2008, DOI: 10.1039/b717861a

The group's method is based on glycine scanning, which compares a peptoid with analogues in which the nitrogen-linked side-chains are replaced with hydrogen. This deletion strategy quickly identifies the side-chains required for biological activity, allowing researchers to strip away any superfluous atoms.

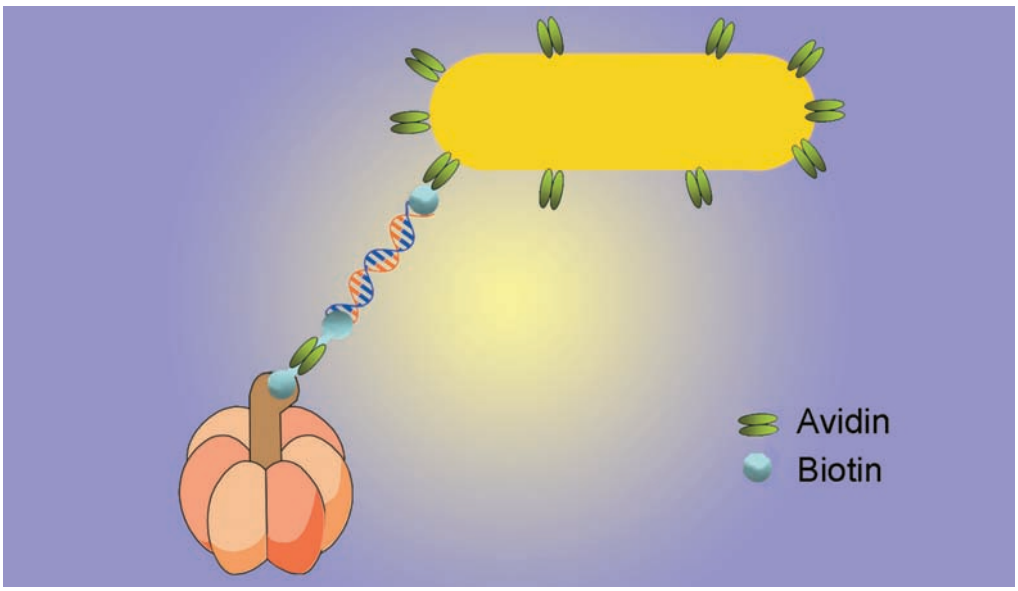
Using this technique, the team created a proteasome inhibitor that was five times more active than the parent molecule in cultured cells. The proteasome is a protein complex that degrades damaged proteins and its inhibitors have been used in chemotherapy to target blood cancers. The researchers attributed the inhibitor's improved activity to the removal of charged residues, which increased the peptoid's cell permeability.

Focusing on the minimal pharmacophore should simplify structure optimisation in drug development, said Kodadek. 'The aim is to quickly cut down the molecule to its essentials,' he explained, adding that 'the next step is to subtly change the essential side-chains to improve the fit of the molecule with the protein target and thus increase its potency.'

Russell Johnson

Enzyme power moves gold nanorods for fast DNA sensing

DNA detection with a twist



US scientists have set DNA detection in a spin by exploiting one of nature's molecular motors.

Wayne Frasch and co-workers from Arizona State University, in Tempe, have used enzyme F1-ATPase as the engine of a new DNA detection device. ATPases catalyse adenosine triphosphate (ATP) decomposition to produce energy. F1-ATPase can use this released energy to spin – it can act as a rotary motor.

Frasch's device works by coupling gold nanorods with F1-ATPases bound to a surface.Two short, labelled DNA strands complementary to a target DNA sequence are added to a DNA sample. If the target DNA is present, the strands bind to it side-by-side, forming a stiff DNA bridge with labels at each end (see figure). The labels used are molecules of biotin (shown in blue), a vitamin that binds strongly to the glycoprotein avidin (shown in green), which is found in egg white. When a solution of the DNA is dropped onto a surface coated with avidin-modified F1-ATPases, the DNA bridges bind by one end to the avidin units using one biotin. An avidin-coated gold nanorod is then bound to the other end of each bridge. The F1-ATPase is made to spin by adding ATP and the gold nanorods also spin, being attached through the bridges. This can be detected simply using microscopy.

Dynamic connection: target DNA forms part of a bridge between molecular motor F1-ATPase (bottom left) and a gold nanorod

The system's detection limit is fewer than 600 DNA molecules in solutions of femtomolar concentrations. Conventional fluorescence-based DNA detection systems have detection limits of only about five picomolar; when fewer targets are present, either multiple fluorescent molecules must be used for each target or DNA amplification, typically using the polymerase chain reaction (PCR), is needed to generate a detectable fluorescent signal. The nanorod sensing method 'avoids the problems inherent to PCR and is much faster than current assays,' said Frasch.

Ulf Landegren, an expert on DNA detection from Uppsala University, Sweden, said, 'the critical question is how the device performs under field or regular lab conditions, where PCR and its related variants have dominated so far.' Frasch admits that he has reported the results from 'clean systems', but his team is now repeating experiments using real samples.

According to the US scientists, their system lends itself to an easy kit-based protocol. But the really exciting thing, said Frasch, is that it is the first practical nanodevice that employs a molecular motor that really works.

Freya Mearns

Reference
J York *et al*, *Lab Chip*, 2008, DOI: 10.1039/b716744j

News in brief

Nanoparticles feel the heat
Nanothermometers for cells could improve an anticancer treatment, say scientists in Puerto Rico.

Peptide potential for cancer imaging
US chemists aim for targeted medical imaging in cancer diagnostics by putting peptide coats on virus shells.

See **www.rsc.org/chembiology** *for full versions of these articles.*

This month in *Chemical Science*

Repulsive microcontainers
Microcontainers made from amino acids and polymers have potential uses in the controlled release of drugs, say German scientists.

Artificial cells mimic ion transport
An inorganic capsule that could be used to study cell functions has been developed by a team of German and US scientists.

Triple action catalysts
Trifunctional organocatalysts that closely mimic natural enzymes can significantly increase reaction rates, say chemists in Japan.

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This month in *Chemical Technology*

Improving enzymes by error
Mutant versions of cytochrome P450 could make for greener chemical synthesis, say UK scientists.

Measuring strontium with a smile
Canadian scientists have reported a non-invasive method to measure strontium levels in human teeth.

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The future of disease detection could be in the balance

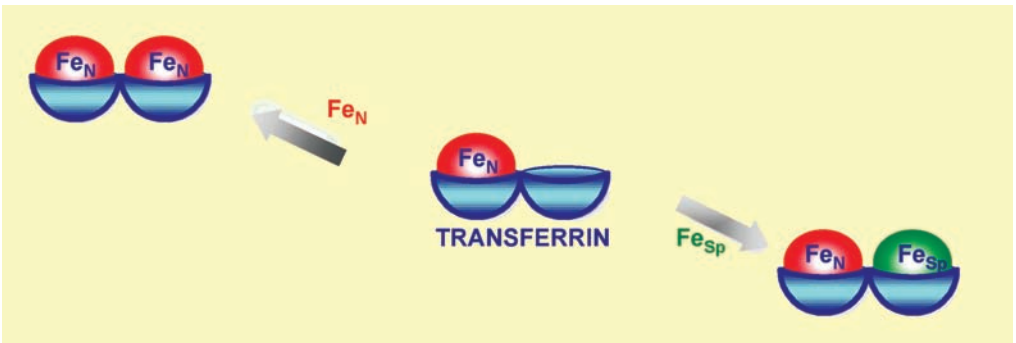
Taking iron measures

A more accurate method to measure iron in clinical samples is proving ahead of its time, say researchers in Spain.

The group at the University of Oviedo, led by Alfredo Sanz-Medel, has developed a technique that allows many variables that can indicate iron-related disease to be measured simultaneously and with great precision.

Any imbalance in the amount of iron in the body can lead to disease, said Sanz-Medel. But many different parameters need to be measured to detect such pathologies – since the metal is used not just as an oxygen transporter in the blood but also in numerous enzymes and processes throughout the human body. Until now these parameters have had to be measured separately, often needing multiple steps.

Sanz-Medel's method avoids this and uses transferrin, a blood plasma protein that transports iron around the body, to measure iron levels in serum. The group saturate the transferrin with either naturally-occurring iron or a non-radioactive isotope and use high performance liquid chromatography (HPLC) and inductively coupled plasma-mass spectrometry (ICP-MS) techniques to measure the amounts of the metal and protein. By comparing the iron isotope ratios, the data can be used to extrapolate clinically useful parameters including the amount of iron bound to transferrin and unbound in serum.



Iron-transport protein transferrin is saturated with natural iron (N) or an isotope (Sp) – the ratios give clinically useful parameters

Group member Maria Montes-Bayón explained the team's approach: 'A great number of biomedical applications use radioactive isotopes. The main advantage of stable isotopes, especially for *in vivo* studies, is that it means no radiation hazard for the patients.'

Zoltan Mester, an expert in using mass spectrometry in isotope ratio analysis, from the Institute for National Measurement Standards in Ottawa, Canada, described the work as a 'dramatically new approach for the study of iron homeostasis.' In fact, the work is so novel that Montes-Bayón admits that the challenge now is to convince the medical community that 'new and more specific tests are necessary to detect increasing numbers of diseases.' With this aim, the group is now looking to start collaborating with biochemists and medical doctors to further the work.

Laura Howes

Reference
M E del Castillo Busto *et al*, *Analyst*, 2008, DOI: 10.1039/b715311b

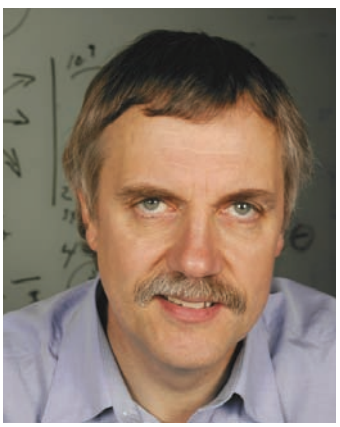
In the current issue of Research Articles...

Read more at www.rsc.org/chembiology

Interview

Putting peptides on the map

Ruedi Aebersold talks to Kathleen Too about proteomics, the PeptideAtlas project and the Trans-Proteomic Pipeline



Ruedi Aebersold

Ruedi Aebersold is professor of systems biology at the Swiss Federal Institute of Technology, Zürich, with a joint appointment at the University of Zürich's faculty of science. He is also one of the founders of the Institute for Systems Biology in Seattle, US. Ruedi is a pioneer in the field of quantitative proteomics and has developed a number of methods that have been widely applied in analytical protein chemistry. Ruedi is a former *Molecular BioSystems* editorial board member.

Why are you interested in systems biology and proteomics?

I have been working in the field of proteomics for a very long time. First, I learnt how to identify and characterise a single protein and then, through technical developments, I started looking at large numbers of proteins.

I am interested in systems biology because I wanted to learn how different systems work and how molecules relate to each other. Systems biology looks at the bigger picture.

Proteomics has got to the point where many protein interactions can be measured. This means there is a lot of useful information for system biologists coming out of proteomics.

What are the most exciting projects you are working on at the moment?

We are trying to find biomarkers that indicate certain diseases. Proteomics itself cannot heal a person but it does have the potential to have a sizeable impact in the pharmaceutical industry. I expect that in the next few years, biomarkers for disease classification will become available, allowing clinicians to detect diseases earlier and treat them more accurately.

Another interest of mine is protein kinases and phosphorylation. It is the most common way to regulate cellular activity. In essence, kinases put the phosphates on proteins and phosphatases take them off. We attempt to establish a relationship between these enzymes and their substrates and determine the functional consequences of protein phosphorylation.

What is the biggest challenge that systems biology should tackle in the near future?

Cancer and obesity need to be addressed. Our work is part of a larger project related to metabolic disease syndrome, partly funded by Roche Pharmaceuticals. The aim is to understand the basic repercussive circuits that lead to type II diabetes and obesity in humans. We work with a consortium of different clinicians and scientists to approach the problem in a more comprehensive way than is possible in a single research lab.

You are one of the founders of the PeptideAtlas project. Can you describe what this is?

The PeptideAtlas project is an attempt to unify in one database all the mass spectrometry-derived protein sequences from a particular species. Many laboratories are doing proteomics by mass spectrometry. They generate a huge amount of data but only use a small fraction of it. We use it to create an informatics database, from which we can learn many things. It tells you which proteins have been identified in any one experiment. It also allows you to start doing analyses of the data to see, for example, how many times has a particular peptide been seen in protein mass spectra. By collecting a community-generated dataset, we hope to get as close as possible to building a complete proteome map.

Which achievement are you most proud of?

We established a computer tool, called the Trans-Proteomic Pipeline, that estimates the percentage error in a dataset. Mass spectometry generates about ten thousand fragment ion spectra per hour. Computer programs match the fragment ion spectra back to a sequence. How do we know that the computer is correct? Many journals, including *Molecular BioSystems*, require that an estimate of error is given when scientists say that they have identified thousands of proteins. Our pipeline enables people to do this and has helped increase the quality of data generated. The software has been downloaded thousands of times and is used in many laboratories. Also, some companies have taken these tools and put them into commercial suites. We have trained several hundred proteomics scientists in the use of the tools.

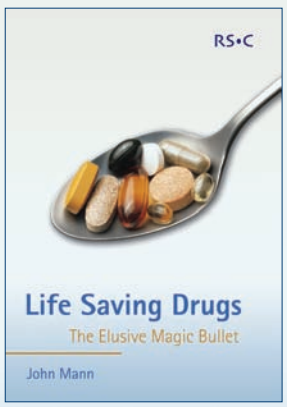
If you went back into the lab, what experiment would you work on?

I think I would work on the relationship between protein kinase and disease because it is clearly important and now technically feasible. Unfortunately, this is highly hypothetical since I can hardly keep up with the other things that need to be done in the office.

Life Saving Drugs

The Elusive Magic Bullet

By John Mann



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Instant insight

Lab on a computer chip

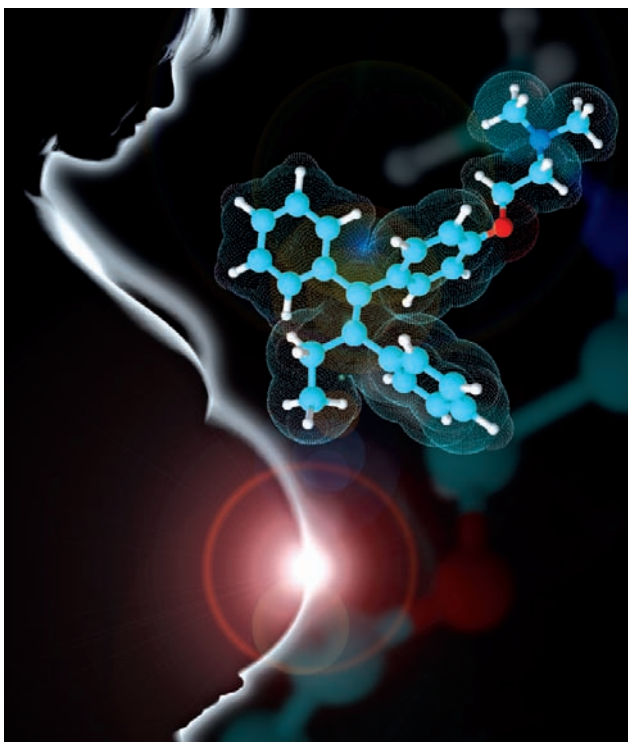
Emilio Benfenati and Alessandra Roncaglioni from the Mario Negri Institute for Pharmacological Research in Milan, Italy, explain why environmental and pharmaceutical chemists should pop into the computer lab

Computers are reshaping the way we explore the life sciences. A palette of *in silico* tools is offering different advantages which could transform environmental and drug research.

What are the advantages of computer methods? Computer experiments are much faster than *in vivo* and *in vitro* ones. Some computer programs can process thousands of compounds simultaneously in a matter of hours, or even less. Computer programs are typically cheaper, in some cases free. But there are also expensive programs, which require skilled personnel. Computer programs do not use animals, which meets ethical concerns about experiments with animals. Computer methods may only require a computer and internet access, making them more widely available than any other method in principle. They do not use chemicals, do not produce chemical waste, and can be used without a sample of the compound to be tested. Indeed, they can be used before the substance has even been made, using only the structure.

What kind of information can computer methods extract? There are different tools, ranging from detailed docking studies, which look at the interactions between drugs and their receptors, to models that examine how structure affects a drug's activity.

In the case of the oestrogen receptor, for example, it is now possible to assess how different compounds interact with the receptor, identifying which chemicals are more likely to bind. This binding is of interest to pharmaceutical companies, interested in new drugs acting through the receptor. Computer programs can also obtain other useful information, such as identifying the part of the molecule that is responsible for a biological effect or its modulation.



An *in silico* experiment: a compound's oestrogen receptor binding properties can be modelled accurately with computers

Oestrogen receptor binding information can also be used in the field of environmental and human protection. The new European REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) legislation requires that each chemical that is produced on the market in an amount exceeding one tonne per year be characterised. This includes chemicals that disrupt the endocrine system – the organs that release hormones, such as oestrogen, in our bodies. Indeed, a series of substances, present in the environment and in our food, can induce activities that disrupt the endocrine system. It would be very useful to identify these chemicals before their marketing and use. Computer methods are attractive for this, potentially providing fast and cheap chemical screening. REACH requirements should therefore boost research on computer models for endocrine disruption effects.

How reliable are the predictions? Computers allow us to predict which substances will have receptor binding properties. This has been shown to be useful for identifying new drugs, reducing the numbers of compounds that need to be screened. However, the prediction is never 100 per cent correct. In predicting potential environmental endocrine disruptors, the main problem is the lack of suitable examples that can be used to provide the correct information. Unfortunately, most of the studies have looked at substances' binding activities, which is only one component of the process that leads to the final effect in the organism. The lack of wider-reaching data makes it difficult to assess the complete process. However, this is a consequence of a broader inadequacy in experiments to assess the phenomenon *in vivo*, which calls for more research in the area.

How useful can computer programs be in the future? A more comprehensive understanding of the endocrine disruptor field requires new perspectives. All sources of information need to be integrated in a more structured process: *in vivo*, *in vitro* and *in silico* studies must be used together to take advantage of the positive features each provides.

Read Benfenati and Roncaglioni's tutorial review 'In silico-*aided prediction of biological properties of chemicals: oestrogen receptor-mediated effects' in issue 3, 2008, of* Chemical Society Reviews.

Reference

A Roncaglioni and E Benfenati, *Chem. Soc. Rev.*, 2008, **37**, 441 (DOI: 10.1039/b616276m)

Essential elements

ChemComm makes an impact

The first in a series of *ChemComm* International Symposia was held, with great success, in China in December. The meeting, on Polymers and Polymer Science, featured a mix of speakers from the UK, the Netherlands, the US and China and was held in three different venues: The Institute of Chemistry of the Chinese Academy of Sciences, Beijing; Fudan University, Shanghai; and Sun Yat-Sen University, Guangzhou.

ChemComm editor Sarah Thomas explained the aim of the symposium: 'The purpose of this event was to bring together scientists in a stimulating and friendly environment that will foster collaborations between the researchers and the universities involved. This was successfully achieved with the first symposium, which was met with an overwhelmingly positive response from all who took part.'

ChemComm editorial board member, and speaker at the symposium, David Haddleton was extremely impressed by the event and what it represents for advancing the chemical sciences. 'The RSC is right to focus efforts on China,' he said, 'my impression is that the Chinese are on the whole very receptive of the UK and the RSC.'

ChemComm is the flagship journal of the RSC, publishing some of the most significant work in the chemical sciences. A long and successful history has seen the journal adapt and evolve to meet the changing publishing environment. Today the journal is the fastest at publishing general chemistry communications.

Building on the success of the first symposium, two more *ChemComm* international symposia are planned over the next 18 months, both likely to be held in Asia.

Watch out for details of these events and other exciting ChemComm developments at www.rsc.org/chemcomm

Journal free for all

RSC Publishing is using a new approach to provide access to *Energy & Environmental Science*, the new journal scheduled for launch in summer 2008.

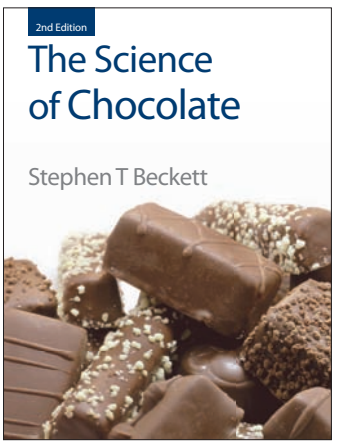
All online content will be available for free during 2008 and 2009. Access, which will be managed by institution and IP address, will be provided following a simple registration process. In addition, the current issue of the journal will be freely available to everyone online, without the need for any registration.

The new approach is in response to feedback from scientists, librarians and other information specialists. The free access will help both scientists and librarians/information specialists to fully evaluate the new journal, before they consider taking out a license or a subscription in 2010.

'We're delighted to launch this new journal in response to feedback from the community,' commented John Haynes, RSC Publishing's editorial director. 'Authors will also benefit from publishing in the journal because the access model is designed to maximise ease of use and global visibility.'

To register for free access at your institution, please complete the online form at www.rsc.org/ees_registration

Hot off the press



First published in 2000 *The Science of Chocolate* has become an international best seller! Widely used in industry and academia throughout the world, *The Science of Chocolate* has even been translated into Spanish and Japanese.

February 2008 sees the arrival of the highly anticipated 2nd edition. Readers will be pleased to hear the 2nd edition has been fully revised and updated: describing the complete chocolate making process from the growing of beans to the sale in the shops. New chapters cover topics such as nutrition, including why chocolate is good for you; how to stop it melting in hot countries; and possible methods of putting bubbles inside a chocolate bar.

A perfect book for chocolate enthusiasts and scientists alike! *For more information visit www.rsc.org/books*

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