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ISSN 1359-7345 CODEN CHCOFS (33) 3409–3500 (2007)

Cover

See Zijian Guo *et al.*, page 3453. Apoferritin has been used to encapsulate anticancer drugs, cisplatin and carboplatin, which has potential to be developed as an efficient strategy for the targeted delivery of the drugs. Image reproduced by permission of Zhen Yang, Xiaoyong Wang, Huajia Diao, Junfeng Zhang, Hongyan Li, Hongzhe Sun and Zijian Guo from *Chem. Commun.*, 2007, 3453.

CHEMICAL BIOLOGY

Drawing together 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

September 2007/Volume 2/Issue 9

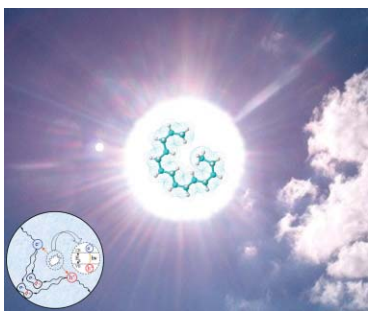
www.rsc.org/chembiology

FEATURE ARTICLE

Photocatalysis: a promising route for 21st century organic chemistry

Giovanni Palmisano, Vincenzo Augugliaro,* Mario Pagliaro and Leonardo Palmisano*

Selective photocatalysis can offer an alternative green route for organics production.



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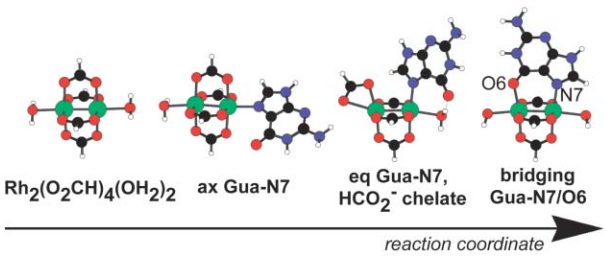
3438

Guanine binding to dirhodium tetracarboxylate anticancer complexes: quantum chemical calculations unravel an elusive mechanism

Dirk V. Deubel* and Helen T. Chifotides

Dirhodium tetracarboxylate complexes are an emerging class of antitumour agents, but their mode of action is not entirely understood. Guanine bases bridge the metal–metal bond *via* N7/O6, but the reaction mechanism remained elusive. Our quantum chemical study unravels this mechanism by prediction of intermediates and transition states.



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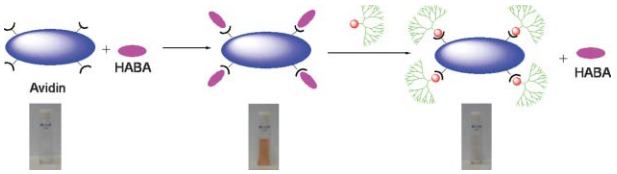
Bioconjugation of biotinylated PAMAM dendrons to avidin

Lei Tao, Jin Geng, Gaojian Chen, Yingjian Xu, Vincent Ladmiral, Giuseppe Mantovani and David. M. Haddleton*

The biotin-terminated PAMAM dendron has been synthesized and the asymmetric dendron used to modify the protein avidin *via* non-covalent bioconjugation.



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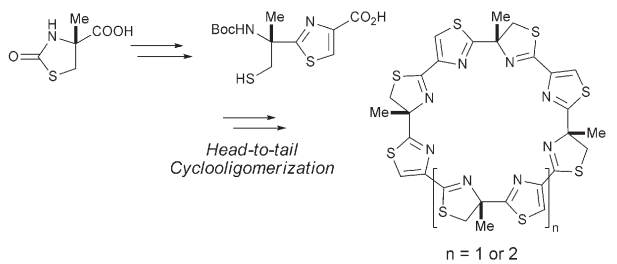
Design and synthesis of thiazoline–thiazole hybrid macrocycles possessing strong binding affinity to Pb^{2+} and Cd^{2+}

Fu She Han, Hidetoshi Tokuyama and Tohru Fukuyama*

Design and synthesis of novel thiazoline–thiazole hybrid macrocyles, along with the application as a new class of selective receptors for metal ions is described. The macrocycle (n = 1) showed strong binding affinity to Pb^{2+} and Cd^{2+}.



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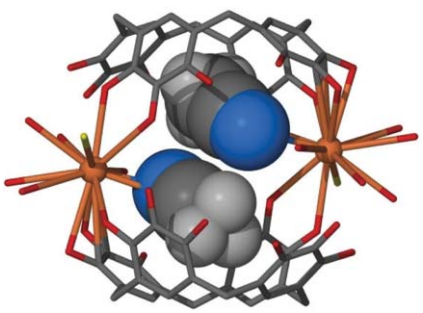
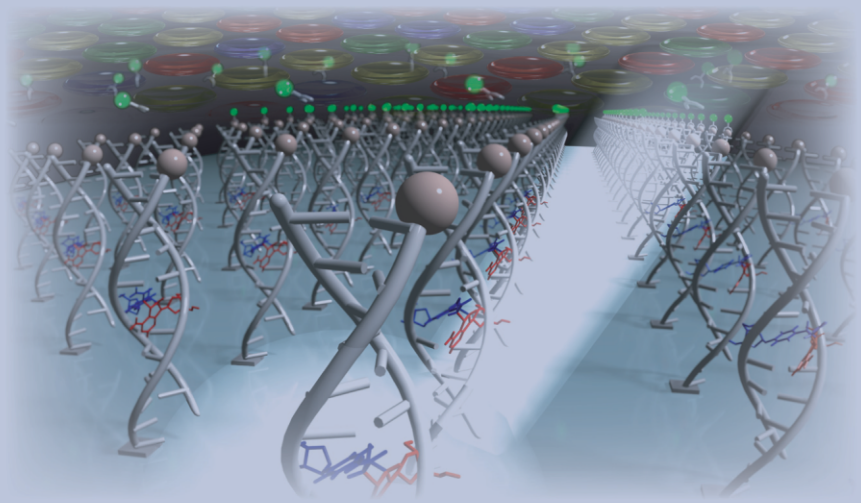
Ionic dimeric pyrogallol[4]arene capsules

Scott J. Dalgarno, Nicholas P. Power and Jerry L. Atwood*

Ionic capsules based on dimeric arrangements of pyrogallol[4]arenes have been structurally authenticated and suggest that there is a degree of flexibility in capsule formation with potential for multiple guest encapsulation and manipulation.





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Forthcoming Articles

Perspective

Virus engineering for bionanotechnology

David Evans, UK

Emerging Area

Palladium catalyzed arylation for the synthesis of polyarenes

Antonio Echavarren, Spain

Articles

Flow and batch mode focused microwave synthesis of 5-amino-4-cyanopyrazoles and their further conversion to 4-aminopyrazolopyrimidines.

Steven Ley, UK

Improved synthesis of O-linked, and first synthesis of S-linked, carbohydrate functionalised N-carboxyanhydrides (GlycoNCAs)

Neil Cameron, UK

Asymmetric synthesis of β^2-amino acids: 2-substituted-3-aminopropanoic acids from N-acryloyl SuperQuat derivatives

Steven Davies, UK

A new azide staining reagent based on "click chemistry"

Stefan Bräse, Germany

Tuning of fluorescence properties of aminoterpyridine fluorophore by N-substitution

Koji Araki, Japan

Enantiospecific synthesis of the heparanase inhibitor (+)-trachyspic acid and stereoisomers from a common precursor

Mark Rizzacasa, Australia

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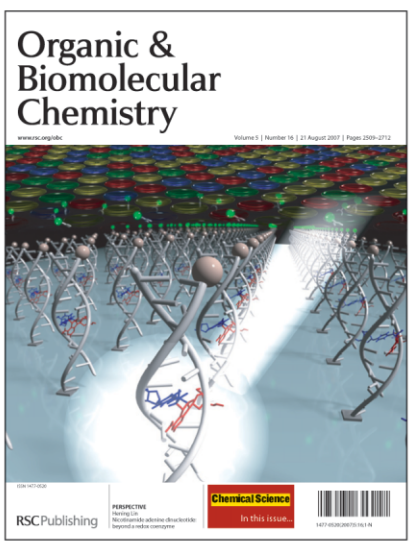

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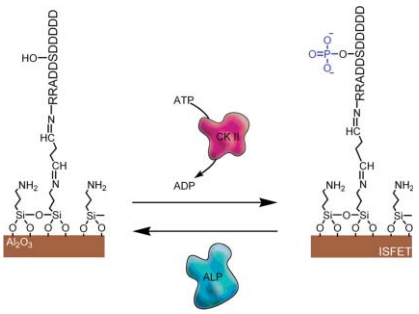
Following a protein kinase activity using a field-effect transistor device

Ronit Freeman, Ron Gill and Itamar Willner*

The specific phosphorylation of a peptide-functionalized ion-sensitive field-effect transistor device by casein kinase II in the presence of ATP enables the electronic readout of the protein kinase activity. Treatment of the phosphorylated surface with alkaline phosphatase results in the regeneration of the active sensing surface.

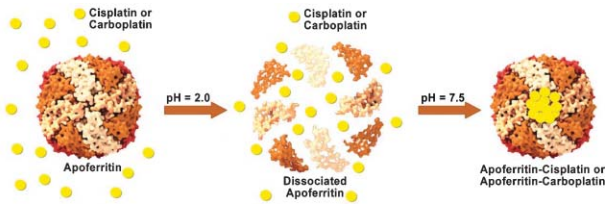


3453

Encapsulation of platinum anticancer drugs by apoferritin

Zhen Yang, Xiaoyong Wang, Huajia Diao, Junfeng Zhang, Hongyan Li, Hongzhe Sun and Zijian Guo*

The anticancer drugs, cisplatin and carboplatin, can be encapsulated in apoferritin. The method may improve the selectivity and toxicity profiles of the drugs and potentially be used for targeted drug delivery.



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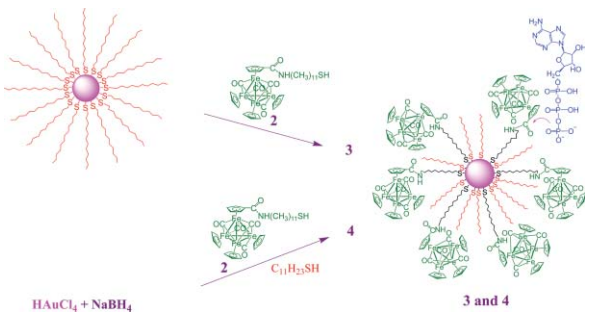
Assembly between gold-thiolate nanoparticles and the organometallic cluster $[Fe(\eta^5\text{-}C_5H_5)(\mu_3\text{-}CO)]_4$ toward redox sensing of oxo-anions

Jaime Ruiz Aranzaes, Colette Belin and Didier Astruc*

Covalent assemblies between the cluster $[Fe(\eta^5\text{-}C_5H_5)(\mu_3\text{-}CO)]_4$ and Au nanoparticles, synthesized using both methods shown here, selectively sense the oxo-anions $H_2PO_4^-$ and ATP_2^-, unlike the amido-Fe_4 cluster alone.

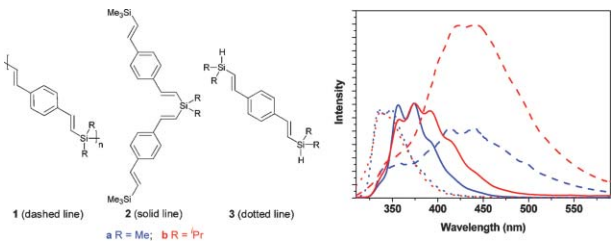


3459

Thorpe–Ingold effect on the conformation and photophysical properties of dialkylsilylene-spaced divinylarene copolymers

Mei-Yu Yeh, Hsin-Chieh Lin, Shern-Long Lee, Chun-hsien Chen, Tsong-Shin Lim, Wunshain Fann and Tien-Yau Luh*

Geminal disubstitution on silicon in dialkylsilylene-spaced divinylarene copolymers may dictate the conformation and photophysical properties of the copolymers.

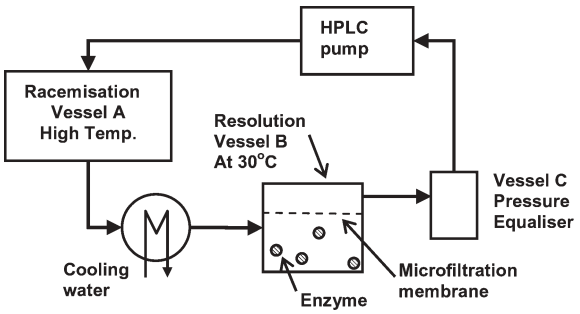


3462

Towards a continuous dynamic kinetic resolution of 1-phenylethylamine using a membrane assisted, two vessel process

Chayaporn Roengpithya, Darrell A. Patterson, Andrew G. Livingston,* Paul C. Taylor,* Jacob L. Irwin and Mark R. Parrett

A continuous process with two separated reaction vessels provides a solution to the problems surrounding the combination of two catalysts in dynamic kinetic resolution reactions.



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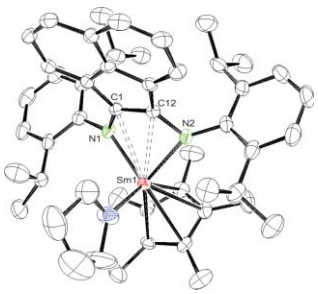
Synthesis and structures of 1,2-bis(imino)acenaphthene (BIAN) lanthanide complexes that involve the transfer of zero, one, or two electrons

Kalyan Vasudevan and Alan H. Cowley*

The number of electrons transferred from the lanthanide to the BIAN ligand depends on the metal, ligand tuning, and ligand bulk.



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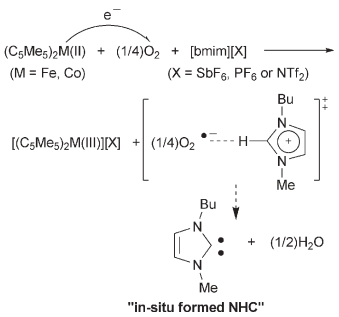
The dramatic acceleration effect of imidazolium ionic liquids on electron transfer reactions

Doo Seong Choi, Dong Hyun Kim, Ueon Sang Shin, Ravindra R. Deshmukh, Sang-gi Lee and Choong Eui Song*

Imidazolium ionic liquids (ILs) exhibited a dramatic acceleration effect on the electron transfer from metal complexes such as $(C_5Me_5)_2Fe$(II) and $(C_5Me_5)_2Co$(II) to the oxygen molecule.



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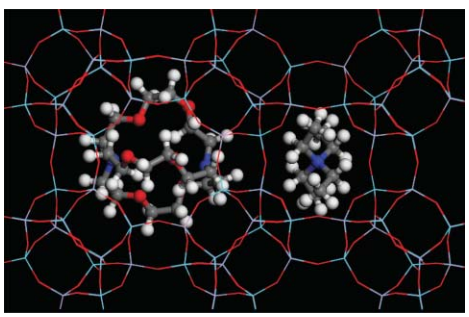
Co-templating and modelling in the rational synthesis of zeolitic solids

Maria Castro, Raquel Garcia, Stewart J. Warrender, Alexandra M. Z. Slawin, Paul A. Wright,* Paul A. Cox, Antoine Fecant, Caroline Mellot-Draznieks and Nicolas Bats

Microporous silicoaluminophosphates with the SAV and KFI framework types have been prepared for the first time, *via* an approach that combines modelling and co-templating.



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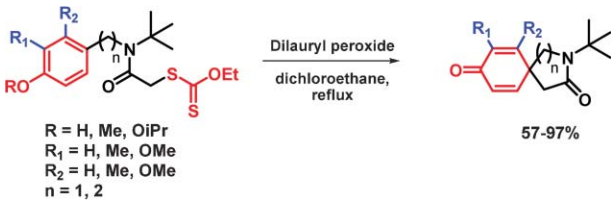
Efficient oxidative radical spirolactamization

Tannya R. Ibarra-Rivera, Rocio Gámez-Montaño* and Luis D. Miranda*

An efficient xanthate-based method for the preparation of azaspirocyclic cyclohexadienones *via* an *ipso* oxidative radical cyclization of *p*-oxygenated *N*-benzylacetamides and *N*-phenetylacetamide is described.



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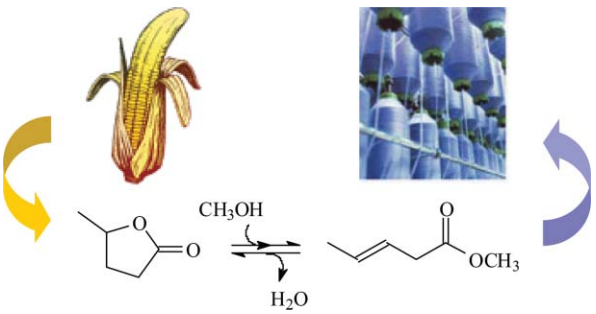
Towards 'bio-based' Nylon: conversion of γ-valerolactone to methyl pentenoate under catalytic distillation conditions

Jean-Paul Lange,* Jan Z. Vestering and René J. Haan

Carbohydrates can be converted to nylon intermediates *via* the formation of methyl pentenoates. We show here that methyl pentenoate can be produced very efficiently under reactive distillation conditions.

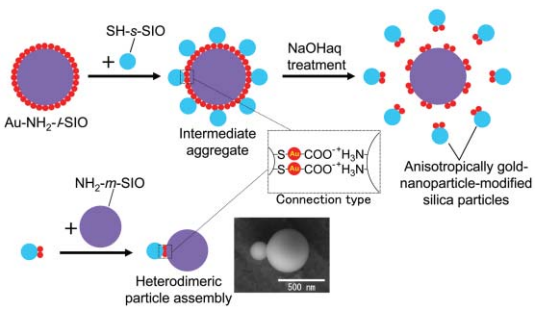


3491

Heterodimeric particle assemblies: Preparation of anisotropically connected spherical silica particles *via* surface-bound gold nanoparticles

Akira Ohnuma, Ryu Abe, Tamaki Shibayama and Bunsho Ohtani*

Assemblies of heterodimeric particles were prepared through selective coupling of two kinds of spherical silica particles of different sizes by connection with gold nanoparticles attached anisotropically to the particles.



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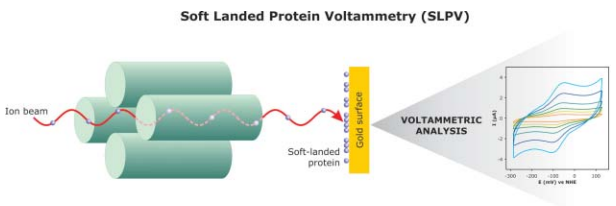
Soft landed protein voltammetry

Federico Pepi,* Andreina Ricci, Alessandra Tata, Gabriele Favero, Marco Frasconi, Stefania Delle Noci and Franco Mazzei*

Ion soft landing offers the possibility of functionalizing surfaces with biologically active molecules. The coupling of this method with voltammetric techniques makes it possible to obtain exhaustive information about the immobilization yield of the deposited protein, the retention of its bioelectrochemical properties, as well as of the nature of the interaction between landed material and the surface.



ADDITION AND CORRECTION

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September 2007 / Volume 2 / Issue 9 / ISSN 1747-1605 / CBHIBN / www.rsc.org/chembiology

Chemical Biology

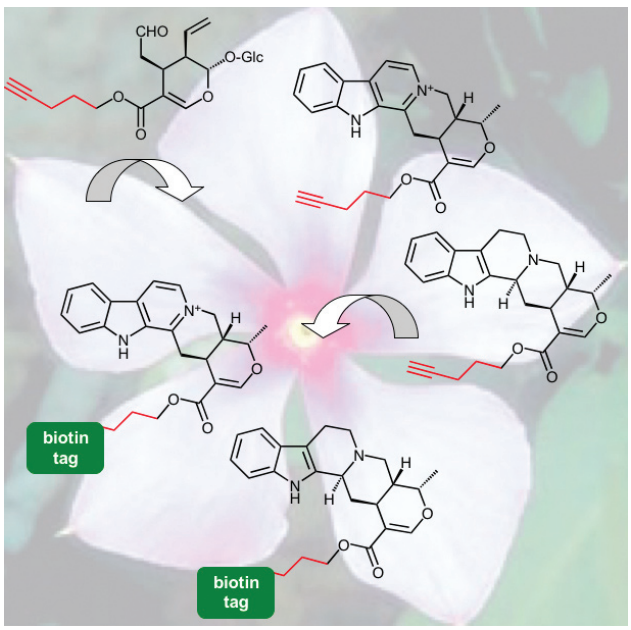
Tagging strategy aids alkaloid extraction from periwinkle cells

Getting a handle on biosynthesis

Artificial plant alkaloids could help demystify biosynthesis.

Researchers at the Massachusetts Institute of Technology, in Cambridge, US, have made tailored alkaloids by feeding periwinkle plant cells with tagged versions of their usual starting materials. The tags can be used to purify the resulting alkaloids and potentially to label plant enzymes along the way, allowing a unique insight into alkaloid biosynthesis.

The team studied the synthesis of terpene indole alkaloids, a family of medicinally important compounds that includes the anticancer drugs vincristine and vinblastine. They started with tagged versions of a key intermediate, secologanin, and found that the plant could process it in the same way as natural secologanin, giving tagged alkaloids. The team could then use click chemistry to modify the tags with biotin, and in turn use the biotin to simplify the extraction of alkaloids from the plant.



Periwinkle cells convert secologanin analogues (top left) into alkaloids

As well as making it easier to identify and purify new alkaloids, this approach could make it possible to find the enzymes involved in their synthesis. 'We plan to use this tag, along with other modified starting materials that we are currently developing, to attempt to label enzymes involved in the terpene indole alkaloid pathway. Then we could use modern proteomic methods to facilitate the identification of the enzymes,' said team leader Sarah O'Connor.

O'Connor explained that investigating natural product pathways is much more difficult in plants than in bacteria, because plant biochemistry is much more complex. 'Plant biosynthetic enzymes are usually not clustered in one place in the genome. Therefore, each enzyme must be individually isolated and then sequenced and cloned, which is a time consuming, arduous process. New strategies to streamline the identification of plant enzymes are greatly needed,' said O'Connor. *Clare Boothby*

Reference
M C Galan, E McCoy and S E O'Connor, *Chem. Commun.*, 2007, 3249 (DOI: 10.1039/b708919h)

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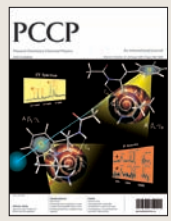


Research highlights

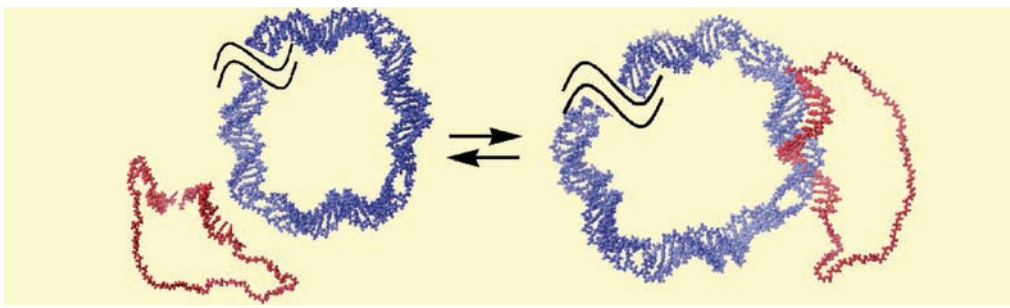
Oligonucleotide padlock protects DNA from cleaving enzymes

A DNA light switch

Researchers in Japan have created a molecular padlock that can lock onto sections of DNA and be unlocked on command. The padlock obstructs DNA-cleaving enzymes and could potentially be used to halt gene transcription.

Kenzo Fujimoto from the Japan Advanced Institute of Science and Technology, Ishikawa, and his colleagues made the padlock by connecting two short stretches of single-stranded nucleic acid with an ethylene glycol linker. One of the two stretches had a vinyl-substituted base at one end. Under light of a particular wavelength, the vinyl group binds to the end of the other nucleic acid, producing a circular molecule sporting a specific oligonucleotide sequence.

The team tested the padlock with a DNA target sequence complementary to that of the oligonucleotide. They introduced the sequence into a plasmid – a ring of double-stranded DNA – and added the oligonucleotide, irradiating the mixture with light. The group found that the oligonucleotide bound to the target sequence and that the bound sequence was not cleaved by DNA-cleaving enzymes, although these acted freely elsewhere on the plasmid. The team was also able to convert the padlock back to linear oligonucleotide by irradiation at a different wavelength, freeing the plasmid.



The padlock (red) interlinks with a DNA plasmid (blue) to form a triple helix structure

Reference
K Fujimoto *et al*, *Chem. Commun.*, 2007, 2968 (DOI: 10.1039/b707524c)

Fujimoto suggested that the technology could also be used to prevent gene transcription. 'Padlock probes can act as inhibitors to block the DNA–protein interaction required for transcriptional initiation,' he said. 'This is not only another tool for photochemists, but also a new development to control gene expression by a photochemical switch.' *Michael Spencelayh*

Device detects oral cancer markers before tumours become visible

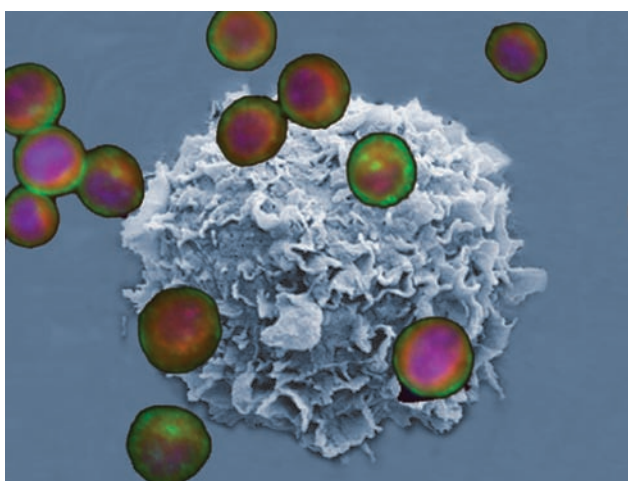
Sifting out cancer cells

A microscopic sieve opens the way to earlier diagnosis of oral cancer, say US researchers.

Worldwide, oral cancer is the sixth most common cancer and is often fatal as many patients are not identified until the cancer is at an advanced stage. Current detection methods rely on the physical identification of a growth, followed by biopsy to identify whether the growth is cancerous.

Now, John McDevitt and co-workers at the University of Texas at Austin have developed a sensor capable of identifying oral cancer at an early stage. The device identifies cancer-related markers, in this case a protein receptor called epidermal growth factor receptor, located on the surface of cells found in saliva and other body fluids. These are present before an obvious tumour is visible.

The sensor is a multi-layer structure on a Perspex base. A cell culture suspension flows through the device, and a membrane within the base acts as a microsieve to capture marked cells before the suspension flows out. Once captured, the cells on the membrane are fluorescently labelled, automatically imaged and analysed. By comparing the labelled sensor to a control, it is possible to detect whether the sample contains the cancer markers.



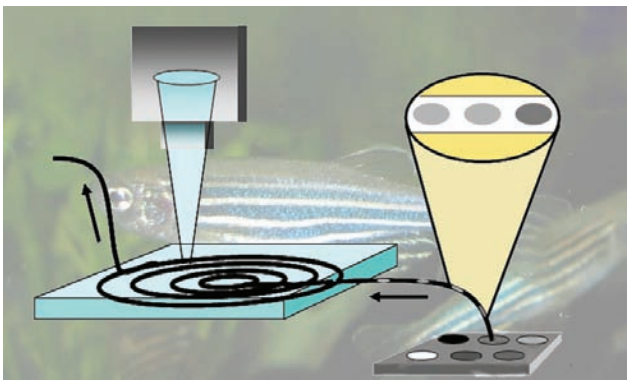
The microsieve membrane captures oral cancer cells

Reference
S E Weigum *et al*, *Lab Chip*, 2007, **7**, 995 (DOI: 10.1039/b703918b)

The new sensor is much quicker than conventional techniques, taking under ten minutes to prepare the samples. It also requires significantly less sample and reagent, reducing cost. This opens the possibility of point-of-care oral cancer screening tools, said McDevitt. He added, 'follow-up visits to follow the progression of the disease after treatment are one area that may be particularly well suited for a portable oral cancer screening unit.'

The team is currently collaborating with the University of Texas Health Science Centre at San Antonio, with the support of the National Institute of Dental and Craniofacial Research Division of the National Institutes of Health, to take the new system into broad clinical use.
Vikki Chapman

Zebrafish hatch screening method



Individual zebrafish embryos grow inside aqueous droplets within a coiled tube

Scientists in Germany are watching zebrafish grow up in a new drug screening technique.

Zebrafish embryos are already used for drug and toxicity testing as they have a number of advantages over other animal models and *in vitro* testing. These include their genetic similarity to humans, low cost and short experiment times, the small amount of drug required and the fact that the transparent embryos can be easily observed. Yet faster and cheaper drug-screening programs are needed to test the large numbers of new compounds that are being synthesised as potential drug candidates.

Now, Michael Köhler at the Technical University of Ilmenau and his colleagues have developed a screening process that could help meet these needs. They used a syringe pump to suck individual zebrafish eggs, surrounded by aqueous medium, into a thin coiled tube filled with a carrier fluid. Each suspended egg was separated from its neighbour by the fluid and an air bubble acting as an oxygen supply.

The researchers monitored and photographed the various stages of the embryos' development using an optical microscope with an integrated digital camera. They showed that the zebrafish eggs can develop and hatch normally within the coiled tube.

The team showed the method's potential for drug screening by using it to test the chemical effects of a detergent on embryo survival and development. Glenn Walker, an expert in biomedical engineering at the North Carolina State University in Raleigh, US, said the work 'is an exciting first step towards what one day may be a fully automated system for screening the toxic effects of compounds on embryos.'

Nicola Burton

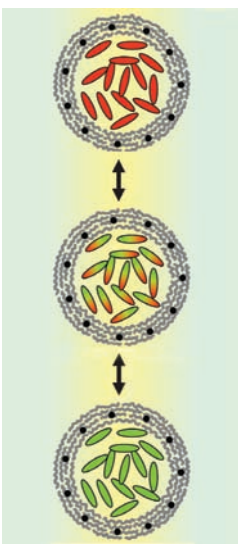
Reference
A Funfak *et al*, *Lab Chip*, 2007, DOI: 10.1039/b701116d

Dyeing to get into cells

Dye-loaded microcapsules that change colour with pH can be used as indicator paper for cells.

Wolfgang Parak, from the Ludwig Maximilians University of Munich, and his colleagues have embedded a pH-sensitive dye in a polymer capsule that can transport the dye into living cells. A colour change in the dye's fluorescence indicates when it has entered a cell and this can be followed by fluorescence microscopy. The change depends on pH: capsules in the alkaline medium outside cells emit in red, capsules ingested by the cells emit in green due to the acidic pH.

According to the German and UK researchers, the capsules could be used in cell analysis, acting as artificial cell components. 'For any kind of cellular diagnostics it would be helpful to have a non-invasive reporter inside cells that constantly measures the concentration of important molecules and sends this information to a detector outside the cell,' said Parak. 'This is similar to the idea of having a miniature diagnosis submarine inside the body, as has been featured in some science fiction movies.'



The polymer capsules turn from red to green as the pH is lowered

Parak says that the capsules need many modifications before they can be used for *in vivo* studies. Eventually though, he envisions them being used to develop a system that detects concentrations of several important molecules inside cells in real time and non-invasively. 'This could be an important tool for diagnostics,' he said.

Elinor Richards

Reference
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News in brief

The measure of cell immortality

US scientists are catching tiny amounts of DNA in a drive to improve testing for enzyme activity linked to tumour growth. In what they call an 'essential step' towards an automated assay for telomerase activity, the team has developed a method to detect as little as 111pg of DNA without having to amplify it.

Neurons grow less dense

A chip that allows neurons to grow in isolation could be used to study how cells communicate. By allowing neuron culturing at low density, the chip could make it easier to measure changes in chemicals between indiviual cells.

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

This month in *Chemical Science*

Cure for Chagas' disease a step closer

Combining chemical and enzymatic approaches brings promise of a cure for a debilitating parasitic disease.

Temperature responsive cell scaffolding

European scientists have developed a porous polymer scaffold for tissue engineering, with tuneable cell adhesion.

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

This month in *Chemical Technology*

Protein detection made simple

A sensitive technique uses colour-changing gold nanoparticles to detect proteins as they bind to DNA.

See **www.rsc.org/chemicaltechnology** *for a full version of this article.*

If you wish to receive an e-mail when the next issue of *Chemical Biology*, *Chemical Science* or *Chemical Technology* is published online, you can sign up to the RSC's e-mail alerting service. To sign up, go to www.rsc.org/ej_alert

Spectrometry provides insight into the more volatile of cancer cell metabolites

Selenium gets the cold treatment

How and do selenium supplements really work? Analytical scientists are helping to find the answer.

Selenium compounds such as methylseleninic acid have known anticancer activity, but the way they work is not well-understood. Now, UK scientists have used analytical methods to study how selenium compounds are metabolised in human cancer cell lines. 'These novel methods will be used in the context of clinical trials investigating selenium supplementation to identify the mechanisms by which selenium exerts its biological effects,' said Heidi Goenaga Infante, at the LGC in Teddington, who fronted the research.

Goenaga Infante and her colleagues used a combination of analytical techniques, including mass spectrometry and gas chromatography, to detect the selenium metabolites. To analyse the volatile metabolites, the team employed a technique called cryogenic oven-cooling gas chromatography, which involves cooling the apparatus rapidly down to temperatures as low as -60 °C.

BIGSTOCKPHOTO

'This method showed advantages in terms of cost and simplicity,' said Goenaga Infante.

The researchers found that *Se*-methylselenocysteine is the major selenium metabolite in lymphoma cell lines treated with methylseleninic acid. They have also reported the first mass spectrometry data for water soluble precursors of methylselenol – a metabolite with anticancer activity – and volatile methylated selenium species formed in the selenium-treated cells.

Garlic or supplements –choose your selenium source; but how does it fare in a cancer cell?

Peter Uden, a US expert in analytical science at the University of Massachusetts, Amherst, said, 'this is among the most innovative and valuable contributions to organoselenium speciation in recent years. Any elemental speciation, not solely for selenium, is accessible to this approach. The ability to sample small cellular samples is a substantial advance and the links between selenocysteine and cell metabolism are key findings.'

In the future, Goenaga Infante says, she hopes to develop methodologies for measuring and identifying analogous sulfur-containing biomolecules in biosamples.

Kathleen Too

Reference

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In the current issue of Research Articles...

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Koji Nakayama *et al*, *Photochem. Photobiol. Sci.*, 2007, **6**, 836 (DOI: 10.1039/b705049f)

Read more at www.rsc.org/chembiology

Interview

Busting tumours

Jenna Wilson talks to Jan Reedijk about the cisplatin-induced kink in DNA, anticancer chemistry and playing the organ

Jan Reedijk

Jan Reedijk is a professor of chemistry at Leiden University in The Netherlands. His research interests are coordination and bio-inorganic chemistry, in particular focusing on metal-containing drugs , homogeneous catalysis and molecular materials.

Your current work focuses on platinum anticancer chemistry. What does this involve?

In the 1960s, Barnett Rosenberg rediscovered the use of cisplatin as a successful cytostatic drug. Since then, a lot of new and exciting chemistry has resulted from several laboratories. Our work focuses on improvements to the chemical mechanism of action of cisplatin. This has led to controlled hydrolysis, transport and binding of the platinum species to DNA, with the majority of it binding at neighbouring guanine bases. This chelation causes a distortion of the DNA, which changes its interaction with proteins. Although the distortion is small, it is significant enough for the DNA not to be recognised by repair enzymes in tumour cells.

Using this style of mechanistic knowledge, several new types of compounds have been developed. We have focused on platinum compounds with a side arm. These were initially made to follow the pathway of the platinum species in the cell. Now we have compounds with a side arm that are also intrinsically anticancer active.

How did you become interested in this area?

It was a project that I started over 25 years ago in my previous job at Delft University of Technology. A PhD student had obtained an individual grant for anticancer chemistry and asked me if I would be willing to supervise his work. At the time, I was investigating the use of heterocyclic ligands with other metals. We combined the project with platinum and published our first papers on platinum anticancer chemistry in the late 1970s. After that, I moved to Leiden, where I was able to really expand the topic, thanks to intense collaboration with colleagues in Leiden.

What else are you working on?

We work on molecular magnetic materials and ion exchange materials. In addition, we have a number of projects involving biomimetic chemistry on structurally unusual compounds, and also projects on homogeneous oxidation catalysis. All our work has transition metals in common along with coordination chemistry of, in many cases, heterocyclic ligands.

If you could go back into the lab tomorrow, what experiment would you do?

I have been asked that question many times and each time I have a different idea. Sometimes I want to do molecular life sciences, sometimes molecular materials. Right now I am highly interested in constructing rigid molecular architectures from coordination building blocks and trying to do catalysis with them.

What achievement are you most proud of?

I am very proud of each completed PhD project. To mention one, our group was the first to discover that platinated-DNA contains a kink. This is caused by the chelation of cisplatin, but it remains double stranded which leaves most of the base pairing unchanged. At the time, almost nobody believed us. It was later proved to be true, which gave us a great sense of achievement.

What do you find most rewarding about being involved in academic research?

Academia allows a lot of freedom, which is something that I enjoy. However, what is most rewarding for me is that each year I receive new talented students. I find myself in a position where I can try to shape and polish them and give them hints to forward their careers. That gives me a lot of satisfaction.

What message do you have for young scientists?

Gorlaeus, the founder of science in Leiden, after which our lab is named, published a statement for young people, which I like to quote – 'on the way to finding the truth, never forget that your teacher is your biggest enemy.'

So, my advice is to try to be unconventional and do not always believe your teachers or the literature!

If you weren't a scientist, what would you do?

I would be a musician; I love to play the organ. When I was finishing high school, I had to decide between music and science. Fortunately, I learnt early enough that I am not technically good enough to make it as a professional organ player!

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The Royal Society of Chemistry provides high quality technical, personal and managerial training for chemical scientists.

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RSC members can attend training courses at discounted rates and non-members will receive free RSC membership for a year. Visit **www.rsc.org/training4industry** to find out more about the 4 Chemists and other training courses.

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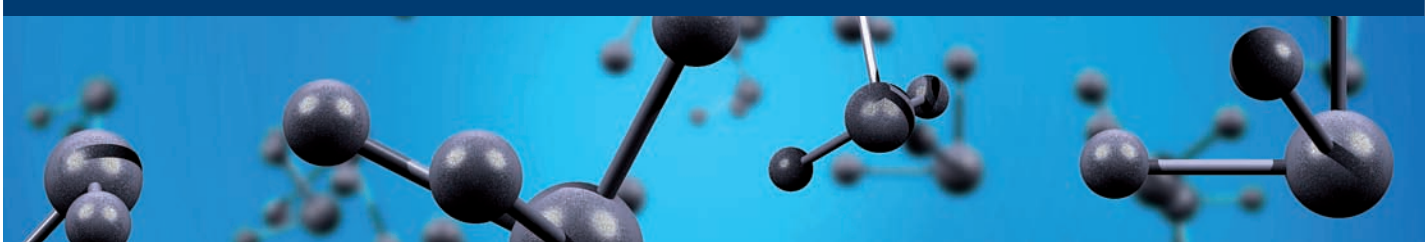

Each year the RSC organises a programme of events dedicated to the advancement of the chemical sciences. With over 30 conferences, one-day symposia and training courses, we offer a range of development and networking opportunities at the cutting edge of science for members and non-members across academia and industry. The centrally organised conferences for 2007 can be found on the RSC website via the URL below.

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Instant insight

Forces of attraction

Jiří Černý and Pavel Hobza at the Academy of Sciences of the Czech Republic, Prague, study the roles non-covalent interactions play in the structure, stability and functions of biomolecules

Chemistry is based on formation and decay of the covalent bond. The bond is one of the most successful concepts in science and it is possible to state that present theoretical and quantum chemistry can fully describe its nature. Biology needs much weaker interactions and covalent bonding clearly does not fulfil this requirement. So, besides strong covalent bonding, nature has been forced to create other, considerably weaker bonds to represent the basic machinery for the very existence of life. These bonds are called non-covalent interactions and their nature is completely different from that of the covalent bond. Non-covalent interactions act between different molecules as well as between parts of a single molecule.

Non-covalent interactions are evident at the macroscopic as well as the microscopic level: they are responsible for a gecko's ability to climb smooth vertical surfaces – even flat glass. Contacts between keratinous hairs, or setae, on its feet and the surface are responsible for surprisingly strong adhesion.

Other examples of non-covalent interactions are less spectacular but more important for nature. Firstly, water – a prerequisite for life. Non-covalent interactions are responsible for the very existence of the liquid phase (and solvation phenomena), but water in particular. Water possesses some very specific properties, such as melting and boiling temperatures, that differ greatly from those of other isoelectronic systems (methane, ammonia). These differences are explained by the existence of specific non-covalent interactions not present in the other systems.

Crossing the scales: non-covalent interactions feature throughout nature, from the folding of DNA to a gecko's ability to climb walls

Secondly, non-covalent interactions are responsible for the structure of biomacromolecules such as DNA, RNA and proteins. It is well-known that a biomacromolecule's function is determined mainly by its structure.

Thirdly, non-covalent interactions play a key role in molecular recognition, one of the most important processes in life. This process ensures extremely high fidelity in information transfer, for instance in transcribing and using the genetic information stored in DNA and RNA.

The unique role of non-covalent interactions in biology is based not only on easy formation of molecular complexes but also on their easy decomposition. For example, DNA should be stiff enough to safely store genetic information, yet simultaneously soft enough to allow it to unwind when the information is to be reproduced. Evolution has evidently selected non-covalent interactions over the too strong (approximately 10–100 times) covalent ones.

While theoretical description of covalent interactions is routine nowadays, description of non-covalent interactions remains one of the most difficult tasks in computational science. Due to their softness, non-covalent interactions are difficult to study theoretically and experimentally, and typically a complete picture is obtained only by combining the two techniques.

Two main interaction motifs (planar hydrogen-bonded and vertical stacked) exist between the building blocks of the most important biomacromolecules: DNA and proteins. The bonding in planar hydrogen-bonded DNA base pairs and amino acid pairs is well understood, but the role of the vertical stacking interactions, their origin and magnitude, was unclear until recently. Only the most accurate calculations of both interaction motifs revealed their relative importance and biological roles. It is now clear, and it is surprising, that it is the stacking that contributes dominantly to DNA stability. Much stronger hydrogen bonding actually destabilises the double helical structure.

The future of molecular biology will be defined by our understanding of non-covalent interactions. Only through these can we truly interpret biological processes at the molecular level.

Read Černý and Hobza's perspective 'Non-covalent interactions in biomacromolecules' in a forthcoming issue of Physical Chemistry Chemical Physics.

Reference
J Černý and P Hobza, *Phys. Chem. Chem. Phys.*, 2007, DOI: 10.1039/b704781a

Essential elements

Five fast and first-rate years

As celebrations for the fifth year of publishing for *Organic & Biomolecular Chemistry* (*OBC*) continue, RSC Publishing staff have been reflecting on the activities and successes.

Launched in 2003, *OBC* was built on the foundations laid by its predecessors *Perkin Transactions 1* and *2*. The intention was to ensure a strong international presence in the organic community – which has already been fulfilled. Not only does *OBC* have a competitive impact factor of 2.874, it also boasts quicker publication times than any of its competitors.

'The achievements over the first five years have been tremendous,' commented *OBC* editor Vikki Allen, 'and with the continued help of our authors, referees and readers we anticipate a first-rate future.'

As part of the celebrations for five successful years of publishing, the journal has featured a series of 'Top 5 articles' from a variety of geographic areas, plus members of the Editorial Board have selected their favourite five articles published in the journal since launch.

Benjamin List, the winner of the 2007 *OBC* Lecture Award, spoke about the challenges for chemists during his lecture on organocatalysis at the 20th International Symposium: Synthesis in Organic Chemistry in July. Whatever the future challenges across the broad organic spectrum of synthetic, physical and biomolecular chemistry, articles published in *OBC* are sure to be at the forefront.

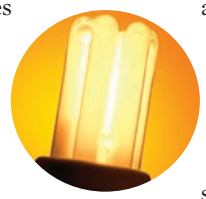
Read more at www.rsc.org/obc

Packed with energy

One of the major challenges for the twenty-first century is the development of cleaner, sustainable sources of energy. The chemical sciences will play a critical role in successfully overcoming such issues, and the RSC is devoted to addressing them and working toward a better, cleaner future.

For more news on energy related research from RSC Publishing, please visit www.rsc.org/energy

Issue 30 of *Journal of Materials Chemistry* hosts a theme issue dedicated to New Energy Materials. Guest edited by M. Saiful Islam (University of Bath, UK) and including contributions from a range of internationally acclaimed authors, the issue highlights some of the latest developments in energy conversion and storage technologies making it a must-have for all scientists interested in energy research.



With the fastest publication rates in the industry and a soaring impact factor of 4.287 (a staggering increase of 58% over the past 2 years), *Journal of Materials Chemistry* has a well deserved reputation for excellence in the field.

Materials chemistry will play a critical role in developing energy-related applications and therefore it is particularly timely to publish a focused set of articles covering this. The issue contains more than 20 articles on a range of topics, including: fuel cells, lithium-ion batteries, solar cells and hydrogen storage, and additionally hosts several feature, application and highlight articles.

Further information can be found at www.rsc.org/materials

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