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## SCIENCE CONCENTRATES

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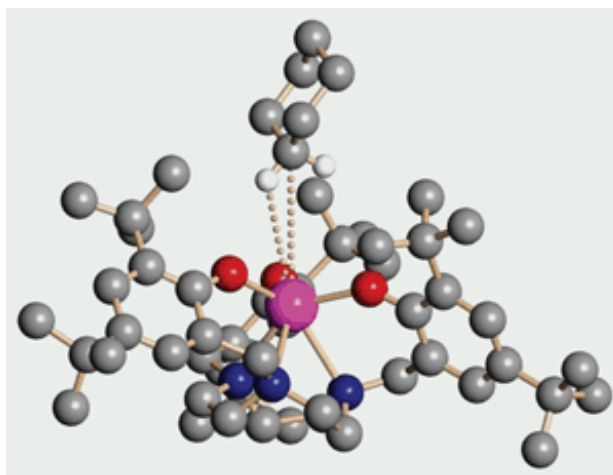
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### Good evidence for stable metal-alkane coordination

Metal-alkane complexes are expected intermediates in catalytic C-H activation processes that lead to new C-C bond formation. These complexes have been examined in computational studies, but experimental data confirming such species are generally limited to fleeting spectroscopic sightings. Chemistry professors Karsten Meyer and Arnold L. Rheingold and coworkers at the University of California, San Diego, now report X-ray diffraction results on a series of alkane adducts of a uranium(III) complex [*J. Am. Chem. Soc.*, **125**, 15734 (2003)]. The experimental data, supported by computational studies, make these complexes the first fully documented examples of stable metal-alkane coordination, Rheingold tells C&EN. The adducts are formed by recrystallizing a tris(hydroxybenzyl)triazacyclononane uranium complex with various alkanes. The X-ray results reveal the connectivity of the alkanes in the U(III) coordination sphere (shown for cyclohexane; red = O, blue = N, magenta = U, white = H). The findings may provide new insight into C-H activation involving transition-metal catalysts.

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## Cell-signaling database launched

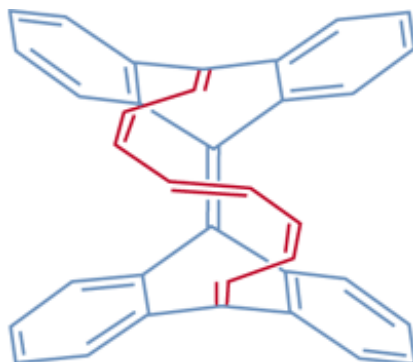
Calling it "a groundbreaking new form of scientific publication," Nature Publishing Group (NPG) and the Alliance for Cellular Signaling, an academic research project, have launched the Molecule Pages, a highly structured online database for proteins that are involved in transmitting and processing signals inside cells. The database, expected eventually to include several thousand different molecules, is a step on the road to creating a "virtual cell"--"a computer simulation of cellular behavior that is close enough to the real thing to reliably predict the responses to treatments and drugs that have yet to be tried in the laboratory or clinic," according to NPG. "This holds the promise of accelerating the pace of [R&D] by orders of magnitude." The Molecule Pages (<http://www.signaling-gateway.org/molecule>) is "a new type of scientific publication" in which invited experts enter what is known about specific proteins, allowing this information to be shared with other researchers much more effectively via the Web. The contents of the database, formally citable using digital object identifiers (DOIs), will be subjected to rigorous and anonymous peer review by NPG. Access to the Molecule Pages is free.

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## First aromatic Möbius molecule

The topology of a Möbius strip, a ring with a half twist, has intrigued chemists as a synthetic target for decades. Making a conjugated Möbius molecule has been of particular interest because theorists speculate that the half twist (seen in the orientations of the p orbitals) would bestow aromaticity on a molecule having  $4n \pi$  electrons, rather than the  $4n + 2 \pi$  electrons usually required for aromaticity. While the Möbius topology has been observed in transition-state species, unstable intermediates, and nonconjugated cyclic molecules, the obligatory twist has made synthesizing a stable aromatic Möbius strip challenging. Now, Rainer Herges and Dariush Ajami at Kiel

University, in Germany, report the first synthesis and isolation, in milligram quantities, of a stable aromatic Möbius hydrocarbon (shown) [*Nature*, **426**, 819 (2003)]. The molecule contains a flexible polyene bridge (red) that twists to connect the ends of a rigid bianthraquinodimethane moiety (blue). As predicted, the structure exhibits moderate aromaticity with 16  $\pi$  electrons.



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### Sensor detects cystic fibrosis

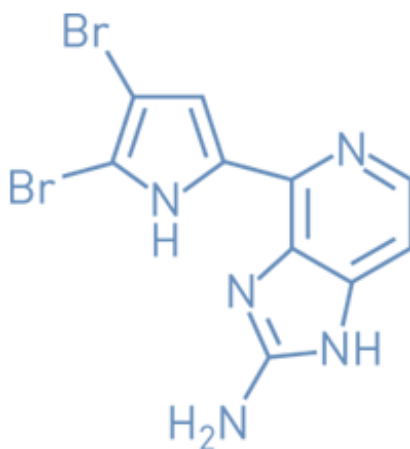
Nanosensors made from silicon nanowires functionalized with peptide nucleic acid (PNA) receptors can distinguish DNA having the mutation for cystic fibrosis from DNA lacking the mutation [*Nano Lett.*, published online Dec. 9, <http://dx.doi.org/10.1021/nl034853b>]. The test takes only a few minutes and can detect the genetic mutation at femtomolar concentrations. [Charles M. Lieber](#), chemistry professor at Harvard University, and his former postdoc, Pennsylvania State University assistant professor Jong-in Hahn, developed the device and chose PNA for the system because it binds DNA with a greater affinity than corresponding DNA recognition sequences. Lieber speculates that a working prototype able to detect the mutation in blood or other bodily fluids could be ready in just a few years. His group has already built an experimental, business-card-sized version of the device. Lieber also thinks that this approach could be used to screen for other genetic diseases and could even be used to thwart bioterrorism by detecting viruses.

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### Sponge yields antiangiogenic agent

Ageladine A, a fluorescent antiangiogenic natural product with an "unprecedented chemical skeleton," has been isolated from a marine sponge, reports a collaboration of Japanese and Dutch scientists. The group, led by professor Nobuhiro Fusetani in the graduate school of agriculture and life sciences at the University of Tokyo, found that the new alkaloid inhibits matrix metalloproteinase 2 (MMP-2). But it does so differently than most known MMP-2 inhibitors, says University of Tokyo coauthor Yoichi Nakao. Most inhibitors are hydroxamate

derivatives that chelate the  $Zn^{2+}$  necessary for MMP-2 activity. Ageladine A pays little attention to  $Zn^{2+}$ . Instead, Nakao suspects that the alkaloid blocks MMP-2 from forming a complex with a group of proteins essential for the "invading front of migrating cells" during angiogenesis and tumor metastasis [*J. Am. Chem. Soc.*, **125**, 15700 (2003)]. The authors predict that the molecule could be a useful fluorescent probe for studying cell migration in angiogenesis and cancer metastasis.



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