

Spotlights on Recent JACS Publications

■ ENHANCED NMR METHOD SPEEDS PEPTIDE ANALYSIS

In dynamic nuclear polarization (DNP), the magnetization of unpaired electrons can be transferred to neighboring nuclei whose NMR signals are then selectively enhanced. DNP in solid-state NMR (ssNMR) spectroscopy has gained much attention recently, especially for biological systems where sensitivity and resolution have long been a challenge due to sample size limitations.

Mark Lorch and co-workers have applied DNP-enhanced 2D ssNMR spectroscopy to studies of a signal peptide bound to the membrane-associated SecYEG complex, a textbook example of using DNP for NMR signal amplification on biological systems that are otherwise inaccessible by conventional NMR methods (DOI: 10.1021/ja209378h).

The SecYEG translocon complex coordinates the transport of proteins through biological membranes, and NMR is a useful technique to obtain high-resolution structural information about the recognition and translocation trigger mechanisms of the complex. With about 32-fold DNP signal enhancement, the researchers were able to acquire 2D NMR spectra in 20 h with excellent sensitivity, resulting in unambiguous assignment of resonances of individual amino acid residues within the complex. In contrast, conventional NMR methods would require weeks or even months to collect the same quantity and quality of data. **Lingling Chen, Ph.D.**

■ ZINC-MEDIATED TRANSCRIPTION REGULATION IN *STREPTOCOCCUS PNEUMONIAE*

In bacteria, the multiple antibiotic resistance regulator (MarR) family of proteins plays a role in everything from regulating virulence factors to resisting antibiotics. To help understand how such proteins work, David Giedroc and colleagues have obtained a 3D structure of the first metal-dependent member of this family, *Streptococcus pneumoniae* adhesin competence regulator (AdcR) (DOI: 10.1021/ja2080532).

AdcR regulates production of several *S. pneumoniae* proteins, many of which are also involved in the microbe's virulence in humans. *S. pneumoniae* can cause a wide array of illnesses, some as mild as sinusitis and others as severe as pneumonia and meningitis. The AdcR protein works to turn off protein production only when the metal zinc binds to it. This allows AdcR to stop the production of the proteins that transport zinc into the cell, until the microbe requires more zinc. If AdcR were unable to repress the production of zinc transport proteins, zinc would accumulate inside *S. pneumoniae*, upsetting the nutrient balance in the microbe and slowing its growth.

The zinc-bound structure of AdcR provides a first glimpse of the mechanics of a MarR protein whose gene-repression action depends upon a metal. Molecules that specifically target AdcR or other proteins involved in virulence or in zinc regulation could provide routes to treating illnesses caused by the respiratory pathogen *S. pneumoniae*. **Kenneth J. Moore**

■ TRAPPING EVASIVE LINEAR TRIPLY BONDED PHOSPHORUS COMPOUNDS

Organophosphorus compounds, containing both carbon and phosphorus atoms, are used for a wide range of purposes, including drug development, pesticides, herbicides, and ophthalmic drugs. Phosphorus compounds with multiple bonds, both double and triple, are often used as precursors for organophosphorus species. In addition, phosphorus triply bonded to nitrogen has been detected in both interstellar clouds and the atmospheres of Jupiter and Saturn, making it particularly intriguing to scientists studying the origin of life.

Helmut Beckers and co-workers recently synthesized the previously undetected O=P≡N linear molecule through the decomposition of O=P(N₂)₃, via photolysis with an ultraviolet ArF laser (DOI: 10.1021/ja2091867). The researchers detected the compounds through infrared spectroscopy in an argon matrix and corroborated these assignments with *ab initio* calculations. They also found that the OPN molecule could interconvert to the ONP isomer through near-UV irradiation.

Understanding this process may help chemists create these multiply bonded phosphorus compounds more easily, leading to more available building blocks for organophosphorus work. Moreover, such gas-phase phosphorus chemistry could help scientists to understand how interstellar elements were incorporated into increasingly complex molecules such as amino and nucleic acids. **Leigh Krietsch Boerner, Ph.D.**

■ A TEMPLATE FOR NANOTUBES

The unusually light weight, super strength, heat resistance, and ultrathin nature of carbon nanotubes (CNTs) could eventually allow electronics to be miniaturized to the nanoscale. But before researchers can reach this lofty goal, they will need to overcome the problem of CNTs' duality: Some CNTs act as semiconductors, but others act like metals with current-carrying capacities 1000 times greater than that of copper wire.

To get around this obstacle, Lawrence T. Scott and co-workers designed a template for only metallic CNTs (DOI: 10.1021/ja209461g). This template has a C₅₀H₁₀ structure with a hemispherical shape and cylindrical rim ideally suited for extending into new nanotubes. The synthesis process starts with the bowl-shaped polyarene corannulene. The researchers chlorinate corannulene and then add on five additional aromatic rings. Rapid heating under air- and oxygen-free conditions stitches together the final hemispherical template structure in reliable 2–3% isolated yields.

The authors anticipate that when methods are developed to elongate nanotubes from these end-caps, gram quantities of pure, metallic nanotubes could be grown from milligram amounts of template. These uniformly templated nanotubes could find widespread utility, possibly in electronic devices, medical technology, or environmental applications. **Christen Brownlee**

Published: January 17, 2012