



# Spotlights on Recent JACS Publications

## BREAKING DOWN BRUCELLA

David Bundle and co-workers dissect key antigenic components of the pathogenic bacteria Brucella, a discovery that will aid in the diagnosis and prevention of brucellosis in animals and humans (DOI: 10.1021/ja5081184). Diagnosis of this highly contagious disease, contracted from unpasteurized milk or undercooked meat from infected animals, relies on the detection of antibodies that bind to carbohydrate-based antigens in the bacteria's cell wall. However, the structural complexity of these antigens has encumbered the development of more effective brucellosis diagnostics and vaccines.

To more definitively characterize Brucella antigens, the authors chemically synthesize a series of six oligosaccharides and conjugate them to proteins. The synthetic glycoconjugates enable detailed examination of specific antibody binding determinants. This characterization leads to the identification of a disaccharide with high potential as a diagnostic tool as well as the design of two novel glycoconjugate vaccine candidates.

Polysaccharides play key roles in immune detection and vaccine development; thus, effective methods to decipher their complex architectures are imperative. This study underscores the power of synthetic organic chemistry to decrypt the intricate nature of polysaccharides and facilitate their exploitation for diagnostic and therapeutic advancement. Eva J. Gordon, Ph.D.

### COMPLEX FUNCTIONALITY FROM DNA BOXES AND POLYMER SNAKES

Hanadi Sleiman and colleagues build on a previously reported method to precisely join DNA segments and synthetic polymers like tinker toys. When snake-like hydrophobic polymers are attached to DNA prisms and cubes, the newly created complex superstructures have potential applications in cancer cell targeting and light harvesting (DOI: 10.1021/ ja509192n).

With a hydrophilic DNA cube head and hydrophobic polymer tail, aqueous mixtures of the structures form spherical micelles. By simply changing the geometry of the DNA cage, the position and number of polymer chains attached to the DNA cage, or the number of repeat units on the polymer, the researchers construct an impressive array of nano-tools. From small groups of DNA cages, to dandelion-like structures, to micelle-dense superstructures, these tools marry the stability and versatility of traditional block copolymers with the programmability and control offered by DNA.

The researchers demonstrate potential applications such as controlled capture and release of DNA cages for drug delivery and dye-based light harvesting. Just as the magic of a building toy lies not within a single brick but in how it combines with others, the significance of this technique is the creative versatility it affords. Jenny Morber, Ph.D.

### FUTURE LOOKS BRIGHT FOR SMALL-MOLECULE-BASED ORGANIC **PHOTOVOLTAICS**

Organic photovoltaics (OPVs) have several characteristics that make them promising as next-generation green technologies, including solution processability, flexibility, and low cost. The primary challenge with any photovoltaic device is achieving a high power conversion efficiency (PCE). Polymer-based OPVs have been demonstrated with PCEs of greater than 10%, but small-molecule-based OPVs (SM-OPVs) have typically lagged behind, with a maximum PCE of 8% reported thus far. But SM-OPVs may have advantages over other kinds of OPVs, such as less batch-to-batch variation, easier energy level control, and more versatile chemical structures, so researchers are not giving up on them.

A new study shows SM-OPVs are catching up, with a new class of solution-processed organic solar cells that have an average PCE near 10% (DOI: 10.1021/ja509703k). Yongsheng Chen and co-workers synthesize and characterize a small molecule, composed of a benzo [1,2-b-4,5-b'] dithiophene central unit with two alkylthiol substitutions. The team then creates bulk-heterojunction solar cells, which they find have an average PCE of 9.60%, the highest PCE ever reported for single-junction OPVs. Modifications to the molecule's structure, coupled with additional efforts toward device optimization, could lead to even greater efficiency, the researchers say.

Christine Herman, Ph.D.

#### METALS GET THE BOOT IN NEW RADICAL POLYMERIZATION METHOD

Metal catalysts are the norm when it comes to atom transfer radical polymerization (ATRP), a common method for creating functionalized polymers with well-defined structure and architecture. But the presence of residual metal is a barrier to the use of these polymers in applications such as microelectronics and biomaterials. Researchers led by Craig Hawker and Brett Fors in collaboration with the Dow Chemical Company set out to tackle this issue by removing metals from the equation entirely, and they now report the first metal-free catalyst system for ATRP (DOI: 10.1021/ja510389m).

The team surveyes a range of possible organic dyes before choosing to explore phenothiazine derivates, which have desirable photophysical properties, cost little, and are easily modified. They find one derivative, known as PTH, that performs as well as an organometallic photoredox catalyst, with the ability to create polymers with low polydispersity and high retention of chain end groups. This new class of metal-free, organic photoredox catalysts makes it possible to use ATRP to produce a variety of functional materials and opens up new avenues for exploration in the fields of small molecule and polymer functionalization chemistry.

Christine Herman, Ph.D.

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