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Spotlights on Recent *JACS* Publications

GLOBULAR PROTEIN BEHAVES LIKE A PUFFER FISH

The standard view that proteins tend to form well-packed, relatively static structures is yielding to a more flexible paradigm. A new twist on this shifting understanding of protein structure and function comes from a study by Chad Petit and colleagues (DOI: 10.1021/jacs.6b12058). The researchers find that a typical globular protein can expand in volume, like a puffer fish, while keeping the same overall shape.

The volume expansion gives the protein more room to move, and a previous study has found that these changes in internal motions are the source of allostery, the transmission of information about protein interactions from the binding site to distant sites within the protein. This study demonstrates that allostery can arise from sources other than canonical structure changes. Moreover, the findings suggest that the definition of the native protein state as a tightly packed globule may need to be revised, allowing for looser proteins that swell and contract to perform their functions. This unexpected observation has broad implications for our understanding of protein allostery, which enables protein function regulations in the cellular environment.
Erika Gebel Berg, Ph.D.

PHYSICAL ORGANIC TOOLS FIND ROLE IN FLOW BATTERY APPLICATIONS

When it comes to intermittent renewable energy sources like solar and wind energy, one of the unmet challenges is large-scale integration into the electrical grid. Redox-flow batteries (RFBs) have been suggested as a potential solution since they can be inexpensively scaled. A class of materials known as redox-active organic materials (ROMs) is attractive as electrolytes for RFBs, given ROMS' relatively low cost, low molecular weight, and high solubility coupled with significant electrochemical potential differences between the anolyte and catholyte. But to be viable for such applications, the materials must also be long-lived in both the charged and discharged states and remain stable throughout electrochemical cycling. Typically, alterations that improve the cyclability of ROMs have concomitantly decreased their redox potential window.

To address this issue, Shelley Minteer, Matthew Sigman, Melanie Sanford, and colleagues apply predictive physical organic tools, which have traditionally been used in drug discovery and asymmetric catalysis, to the development of new battery materials (DOI: 10.1021/jacs.7b00147). The team rapidly identifies a new energy storage material with a combination of high stability, excellent cyclability, and low reduction potential. The researchers are optimistic that the tools may be applied to the design and optimization of new ROM derivatives for RFBs and other electrochemical devices.
Christine Herman, Ph.D.

APTAMERS: MOLECULAR PROBES FOR BIOMARKER DISCOVERY AND VALIDATION

Aptamers are single-stranded oligonucleotides that are created using an iterative technology known as Systematic Evolution of Ligands by Exponential Enrichment (SELEX). The process can be tailored to yield high-affinity aptamer probes, which result when oligonucleotide strands fold into higher-order structures that selectively bind to desired targets—in the same manner as a protein-based antibody, and oftentimes with comparable affinity. Owing to these properties, aptamer probes have the potential to serve as molecular tools for the discovery and validation of disease biomarkers, which is an essential step in the development of new diagnostic tools in personalized medicine.

In a Perspective, Weihong Tan, Liping Qiu, and co-workers provide an overview of the advanced chemistry of aptamer molecules and the critical role they play as molecular probes in biomarker studies (DOI: 10.1021/jacs.6b10646). They explore the use of aptamers in biomarker targeting, the importance of cell surface biomarkers, and the creation of multiplexed biomarker discovery platforms that can increase throughput and efficiency. The authors highlight several major advancements of aptamer-based biomarker discovery strategies and discuss their potential contribution to the field of precision medicine.
Christine Herman, Ph.D.

NEW WAY TO SEPARATE STYRENE FROM ITS PRECURSOR

Styrene is an important feedstock in the chemical industry, key for creating thermoplastics, synthetic rubbers, and resins. It is mainly produced by dehydrogenation of ethylbenzene; however, separating styrene from the large portion of unreacted ethylbenzene through conventional methods is energy-intensive. Further, the two molecules are similar in size, making it difficult to find suitable porous materials for separation. Feihe Huang, Andrew Cooper, and co-workers develop a novel, energy-efficient way to purify this important compound through a crystallization separation using a host molecule with a marked preference for styrene (DOI: 10.1021/jacs.6b13300).

The researchers test two different types of pillar[*n*]arenes (*n* = 5,6), pillar-shaped macrocyclic molecules known to be hosts that can adsorb other molecules. Crystallization experiments show that one of these, pillar[6]arene, demonstrates a strong selectivity for styrene over ethylbenzene. A single adsorption–crystallization cycle yields styrene with a purity of more than 99%, demonstrating the utility of this host molecule. Further investigation shows that pillar[6]arene can be used for multiple purification cycles with no loss of performance, suggesting the material can "self-heal" upon each recrystallization. Future work, the authors note, will focus on increasing the uptake capacity and adsorption kinetics of this promising molecule.
Christen Brownlee

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