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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
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Spotlights on Recent *JACS* Publications

PHYSICOCHEMICAL CLUES TO GENE FUNCTION

Messenger RNA (mRNA) and transfer RNA (tRNA) are essential molecules in protein-production machinery: mRNA serves as the molecular blueprint that guides protein production, and tRNA translates mRNA into proteins by joining amino acids according to the mRNA sequence. Chemist Bhyravabhotla Jayaram and graduate student Garima Khandelwal have developed a computational method based on DNA's physicochemical properties that can predict whether a gene sequence codes an mRNA or tRNA, without the need for structural data (DOI: 10.1021/ja3020956).

The researchers gathered more than 1,500 prokaryotic genomes from public databases, with more than 2 million mRNA and 50,000 tRNA sequences. They used solvation energy as a measure of DNA's ability to interact with water and calculated for each genome the average solvation energy for each pair of neighboring nucleotides of all RNA sequences in that genome.

tRNA solvation energy values are distinctly higher than and readily differentiated from those of mRNAs when comparing the relative solvation energies for all of the RNAs in each of the genomic sequences. This computational analysis of the physicochemical characteristics of the gene sequences reflects the final structures for which they code—tRNAs are stable structures and less-well solvated than mRNAs. This solvation energy analysis offers a new tactic to identify tRNA-coding regions in a genome sequence without needing tRNA's final structure, bringing a new tool to gene-function studies. **Kenneth J. Moore**

COOPERATION YIELDS GREAT RETURNS

Yonggui Robin Chi and co-workers combine both N-heterocyclic carbenes (NHCs) and Lewis acids, effecting cooperative catalysis in order to cleave C−H bonds up to three carbons away from an aldehyde activating group (DOI: 10.1021/ja303618z). NHC catalysis has more commonly been used to functionalize bonds zero, one, or two carbons away from this type of activating group.

Chemical compounds that could be useful in synthetic, analytical, or other practical applications may have reactive and readily functionalized activating groups, as well as less reactive portions of the molecule. A poorly reactive C−H group, for example, may need to be functionalized to make the compound more useful, but this reaction can be difficult when the bond is remote to the activating group.

Using an NHC in combination either with the Lewis acid scandium(III) triflate alone or with magnesium(II) triflate as well, the researchers were able to activate a carbon three positions away from the activating group. After further reaction, they constructed 6-membered lactone rings that are important flavor and aroma constituents in many natural products. The authors were able to achieve good stereochemical control, and they suggest that this cooperative catalysis technique might be useful for selectively and asymmetrically modifying other molecules. **Christen Brownlee**

MOLECULAR DAMS SPEED UP PROTEIN ENRICHMENT

Miniaturized systems that rapidly detect minute quantities of biological molecules with great sensitivity could be game-changers in medical science. These micro- and nanoscale systems have the potential to be used as diagnostic devices to detect diseases at preliminary stages, as well as discovery tools to find new clinically relevant biomarkers. But a major hurdle in developing these systems is picking out the molecules of interest from complex biological samples and concentrating them in one location for detection.

Now Kuo-Tang Liao and Chia-Fu Chou demonstrate an electrokinetic technique that can quickly concentrate traces of a protein at a single location (DOI: 10.1021/ja3016523). They created an array of nanoscale constrictions that work like molecular dams. The nanoconstrictions enhance the local electric field by 10^5-fold over the amount of applied field. Proteins, depending on their size and dielectric responses, get trapped at these nanoconstrictions.

To demonstrate their technique, Liao and Chou tested a fluorescently tagged streptavidin protein molecule and achieved a 10^5-fold enrichment in less than 20 s. The investigators say their approach is significantly faster than most other reported methods, and they suggest that their molecular dams may be particularly suitable in miniaturized devices designed for early disease diagnostics or general protein assays. **Rajendrani Mukhopadhyay, Ph.D.**

NEW STUDY REVEALS SYNTHETIC PRINCIPLES UNDERLYING ORGANIC SEMICONDUCTORS

Researchers led by John Reynolds report synthetic principles that can be used to strategically design π-conjugated polymers for applications in a wide range of semiconductor technologies (DOI: 10.1021/ja301898h).

Organic, π-conjugated semiconductors have been widely applied in recent years as thin-film transistors, as well as sensors and photovoltaic devices. When it comes to designing organic molecules for semiconductor applications, desired characteristics include ease of processing in solution, good charge-carrier mobility, a wide optical absorption profile, and long-term environmental stability. But depending on the desired application, some of these characteristics are more important than others. Hence, organic semiconductors designed for a specific application tend to not be effective enough for applications in other devices, limiting the material's broad usefulness.

The research team performed a comprehensive study to determine the interplay between the molecular structure and the performance of copolymers—made of alternating units of electron-rich and electron-deficient repeats—in both thin-film and photovoltaic devices. They found correlations between the charge transport ability of an organic semiconductor material and its repeat unit structure, molecular weight distribution, and

Published: June 12, 2012

dx.doi.org/10.1021/ja305430t | *J. Am. Chem. Soc.* 2012, 134, 10307−10308

the nature of the solubilizing side-chain substituents, meaning that in the future organic semiconductors could be more easily tailored for specific applications. **Christine Herman, Ph.D.**

dx.doi.org/10.1021/ja305430t | *J. Am. Chem. Soc.* 2012, 134, 10307−10308