

Welcome to ACS Combinatorial Science

It is interesting to contemplate a tangled bank, clothed with many plants of many kinds, with birds singing on the bushes, with various insects flitting about, and with worms crawling through the damp earth, and to reflect that these elaborately constructed forms, so different from each other, and dependent upon each other in so complex a manner, have all been produced by laws acting around us.

These laws, taken in the largest sense, being Growth with Reproduction; Inheritance which is almost implied by reproduction; Variability from the indirect and direct action of the conditions of life, and from use and disuse: a Ratio of Increase so high as to lead to a Struggle for Life, and as a consequence to Natural Selection, entailing Divergence of Character and Extinction of less-improved forms.

Thus, from the war of nature, from famine and death, the most exalted object which we are capable of conceiving, namely, the production of the higher animals, directly follows.

Charles Darwin, *The Origin of Species*, 1859

A century-and-a-half ago, without understanding life's modular or molecular nature, Charles Darwin intuited the central concept of combinatorial science: in the competition between multiple candidates is great power to produce advantageous outcomes. For chemists, the combinatorial enterprise's conceptual home just a decade ago was in drug discovery, and the first roof over its head was the *Journal of Combinatorial Chemistry*. The initiative came from Founding Editor Tony Czarnik, and the journal has thrived under his prescient leadership.

Since then biology has become more molecular in understanding, and chemistry more biological in application. Vibrant advances in pharma have new cousins, from discoveries made by phage display and other “test-tube evolution” procedures, to the multivariate optimization of properties in polymeric materials.

Great changes occurred during Darwin's life as well. With the Market Revolution, he saw subsistence and bartering evolve into buying and selling with money. Cities erected covered markets for shopkeepers to store their goods: Covent Garden was built the year before the Beagle sailed. Being gathered under one roof induced competitors to innovate, and customers received better value when they became selectively discriminating. The participants learned from each other, dramatically expanding their ability to leverage new goods and processes into greater value, giving birth to a new type of society.

With this issue, we introduce a new incarnation of *Journal of Combinatorial Chemistry*, renamed to highlight an expansion of the journal's coverage that will become increasingly apparent in the coming months. Drug discovery will maintain its important

presence in the journal, even as we embrace a new mission:

ACS Combinatorial Science will publish outstanding work that describes or aids the development of molecular function by combinatorial means.

Our definitions of these terms reflect the journal's broader scope:

“Molecular” entities include compounds of all sizes from small molecules to macromolecular materials, exhibiting their key properties alone or as part of a system.

“Combinatorial” methods encompass: synthesis and screening of discrete or virtual libraries of chemicals or materials; diversification and selection of biomolecules by biological methods; and true evolution of molecular systems in vitro or in vivo.

“Outstanding work” is research that we think will broaden and energize investigators in other fields while it defines the state of the art to the specialist.

“Function” is the payoff, the desired outcome of the particular study, and can therefore be extraordinarily diverse. A central theme of *ACS Combinatorial Science* will be the tackling of important problems that challenge our understanding and defy our ability to predict effective answers.

Combinatorial science is an exercise in humility, in which we ask our molecules to teach us their lessons. It is often frustrating, as we learn by trial and error to speak the molecular language. But it is also an opportunity for joy, when unanticipated answers emerge and insights are gained. Most important, it is, as Darwin intuited and many others have shown, the very best way, often the only way, to achieve desired or novel functions in complex situations that matter.

Combinatorial and evolutionary molecular science may be regarded as a new discipline, with many opportunities for cross-fertilization in techniques, as well as limitless potential applications. Our goal is to provide a scientific Covent Garden for a large and diverse group of investigators working in chemistry, biology, and materials science, who may peddle different wares but use a common combinatorial currency. In welcoming your contributions to the journal and your feedback on how we can enhance the publication, I invite you to help make *ACS Combinatorial Science* the first and best home for an integrated view of this exciting new world.

M.G. Finn
Editor-in-Chief

Published: January 10, 2011