

Editorial

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Editorial

Combinatorial chemistry ("CC") is a field in which new chemical substances—ranging from pure compounds to complex mixtures—are synthesized and screened in a search for useful properties. In one sense, chemists have employed an 'empirical' search for properties dating to the alchemists. However, in the past several years some chemists have applied their intellectual creativity to invent new, much more efficient ways of making new substances in ways that facilitate their screening.

Many of the issues raised by this new community of chemists are very often not shared by existing Chemistry communities. For this reason, local communities (e.g., chemists at one company) have worked to create solutions in near isolation. It seems clear that a more global community of chemists facing similar issues would achieve solutions faster. And this is a worthy goal, because the combinatorial search for useful chemical substances portends quality of life improvements that have always been important in maintaining Chemistry's high status.

This community also will benefit from the setting of conventions by a panel of experts. For example, there currently exists no guidelines for the level and type of sample characterization that are both of use to readers and achievable. If one today synthesized a library of 10,000 samples of organic compounds, it would not be feasible to obtain NMR spectra on all samples—the standard required for publication in *The Journal of Organic Chemistry*. However, having no requirement for NMR characterization is an invitation to error and even abuse. A standard must be set, and the Editorial Advisory Board of the *Journal of Combinatorial Chemistry* would assume that responsibility and enforce the decision. It is also true that this must be a living convention; in the face of new technology making high-throughput NMR more accessible, new standards for library sample characterization would be required. Such changes are certain to be required.

Because the goal of this field is worthy and the field itself likely to afford progress, Combinatorial Chemistry as a discipline is not going to go away. All these things support the proposal for a journal as the community's organ for the dissemination of research results.

It is interesting for me to reread this Rationale from the original proposal for the creation of the *Journal of Combinatorial Chemistry* (JCC). At the time of its writing, there was an element of faith required. Today, with so many people engaged in the field, it is apparent that faith was well-placed. The creation of a new Gordon Research conference on 'Combinatorial Chemistry' supports that view.

As an organ for the dissemination of research results to the Combinatorial Chemistry community, JCC must meet the needs of that community. The Associate Editors and Editorial Advisory Board have struggled mightily over the past nine months to define that need. Our discussions have

caused us to ponder, sometimes heatedly, some rather important questions. What makes a piece of work in this field significant? What level of characterization is required to publish a library synthesis? How pure must the products of a library synthesis be in order to publish the results? What methods of purity determination are really useful? The answers to these and many other questions are to be found in the JCC "Notice to Authors"; as a member of this community, I encourage you to read through this document, and then let me know if you think we did a good job.

One of the most significant items we concluded was of great importance to me. Results reported in this Journal are

likely to be replicated in many laboratories. In order to facilitate that replication, experimental detail is essential. Thus, every paper published in JCC has an associated Experimental Section in the print and/or Web versions. Because the traditional Communication or Letter format carries a sense of special urgency and because neither includes an Experimental Section for most chemistry journals, a lack of experimental detail has become equated with special urgency for many chemists. Our group of Associate Editors and Advisory Board members concluded that this was not the right approach for the reporting of combinatorial chemistry experiments. I am still completely convinced that this is the right decision. As future authors, I ask each of you to help us meet the goals of this Journal by taking the time to provide details of your work. It is the best way to make progress as a community.

There are many people to thank. Jack Ochs and Cheryl Shanks of the ACS were supportive of JCC from the very

beginning, as have ACS's Mary Scanlan and Bob Bovenschulte. Anne O'Melia, Diane Needham, and Debbie Cecotti from ACS's Columbus office and Dawn Hayes, Patrick Braswell, Rhonda Rawlings, and Paula Commodore from the Washington office have worked very hard on this project. *The Journal of Organic Chemistry* and *Journal of Medicinal Chemistry* Editors and staff have been of great assistance. JCC is the first 100% ACS journal in eight years. Everyone at ACS who has seen this through from vision to resource can be rightfully proud of their involvement. Now it is our job to make sure that JCC provides a service to Chemistry worthy of ACS affiliation.

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Editor

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