

A new look for chemical information

***Nature Chemical Biology* is committed to enhancing interdisciplinary communication and features online content to increase the accessibility of chemical information for our readers.**

The adage that “a picture is worth a thousand words” is a truism for chemists. In many fields, precise terminology is adequate to describe specific concepts or entities; however, in chemistry, elaborate chemical nomenclature often is not an efficient way to communicate about complex molecules. As a result, chemists have developed shorthand notations to represent molecular information, such as two-dimensional skeletal line drawings for chemical structures and specific arrow notations to illustrate chemical reactivity. These chemical renderings remain the most common ‘language’ whereby scientists ‘speak chemistry’ at the blackboard and in the scientific literature. Chemical biology relies heavily on these structural formulas to describe the relationships between chemical and biological systems, but the field faces the challenge of translating the meanings of these chemical symbols across traditional disciplinary boundaries. To foster the exchange of information by scientists working at the interface of chemistry and biology, the *Nature Chemical Biology* team has developed new ways to enhance the accessibility and utility of the chemical compound information in papers published in the journal.

Most published chemical content is traditionally contained in the schemes, figures and tables of scientific papers. Authors also use abbreviations, acronyms or numbering schemes to identify specific molecules. Though these shorthand notations simplify the presentation of chemical information, they tend to make chemical papers less accessible to the general reader. This is a concern for chemical biology articles, which are intended to attract an interdisciplinary audience. Moreover, since the advent of the Internet, the way by which scientists acquire scientific information has changed. Though some scientists continue to read journal articles in print, most turn to the online HTML and PDF versions of published manuscripts. This expanded use of electronic resources offers an excellent opportunity to make chemical information more accessible and user-friendly to readers of scientific papers.

To take advantage of these opportunities, we have developed several online features that expand the usefulness of chemical compound information for *Nature Chemical Biology* readers (see for example http://www.nature.com/nchembio/journal/v3/n6/compound/nchembio883_ci.html). In all original research papers, compounds that are relevant to the background or results of the paper are assigned a bolded, Arabic numeral that serves as a unique identifier for the compound. Each numerical abbreviation in the HTML and PDF versions of the article is linked to a Compound Data page, which shows the structure and the IUPAC or common name of the chemical compound. From there, readers can download a ChemDraw file of the compound, view a three-dimensional rendering of the molecule (see below), or link to more information about the compound in PubChem (<http://pubchem.ncbi.nlm.nih.gov/>; see *Nat. Chem. Biol.* **1**, 63, 2005 for more information). To provide readers with rapid access to all of the chemical compounds discussed in an article, we feature a Compound Data Index page, which is accessible from the Compound Data page, the

table of contents entry for the paper, and the navigation tools on the right side of the *Nature Chemical Biology* website. Taken together, these features highlight chemical information in a format that is not available in more traditional presentations of chemical content.

Though line drawings offer a useful way to represent molecular structures, chemical compounds exist as three-dimensional objects with distinct conformational preferences. To highlight these properties, *Nature Chemical Biology* has launched new online functionality that permits the three-dimensional visualization of the numbered compounds in each article. Each compound’s 3D page is accessible through the Compound Data pages and provides a three-dimensional rendering of the molecule as an energy-minimized (MM2) conformer. Users are able to rotate, zoom and manipulate the compound in three dimensions on the journal’s webpage. Although the technology is in its infancy, we hope that it will encourage readers to consider the importance of three-dimensional molecular structure in biology.

By adopting a standard chemical style at the journal, we hope to enhance the clarity of how we communicate chemical information throughout our pages. We view this process as a partnership between authors and editors. Authors ensure that the chemical compound information within their papers is complete, scientifically accurate and appropriately formatted. The editorial team recently created two resources to help authors format their chemical structures and expedite publication: a Chemical Structure Style Guide (<http://www.nature.com/nchembio/authors/submit/chemicalstyle.pdf>) that contains a summary of how chemical structure imagery is presented in the journal, and a ChemDraw settings file (<http://www.nature.com/nchembio/authors/submit/NatChemBio.cds>) that authors may apply to render their structures in our preferred format. To support the online chemical content, authors also contribute two files with their final manuscript that the editorial team uses to deposit the study’s chemical information into PubChem, generate the compound information pages and create the three-dimensional renderings of the chemical compounds in the online version of each paper: (i) a formatted ChemDraw file that contains the structure of each numbered chemical compound grouped with its corresponding number, and (ii) a tab-delimited text (or spreadsheet) file in which each compound number is associated with its IUPAC or systematic name. Although authors need to invest additional time in creating these files, their efforts greatly enhance the content of their published papers.

We believe that the chemical content of *Nature Chemical Biology* papers shows how online resources can be used to enhance the accessibility and utility of chemical content in scientific papers. We seek your evaluation of what we have done so far. We would also like to hear your ‘wish list’ for new chemical or biological functionality that will foster communication and collaboration between researchers at the interface of chemistry and biology. ■