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Incorporating chemical structures into scientific figures

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Abstract

Of great import for biochemistry articles is the inclusion of chemical structures in figures; they are common for showing reactions, detailing protein side chains and modifications, and depicting chemical probes. In this ninth installment of the TrendsTalk Special series: Scientific figure development, two scientists share their thoughts: what aspects do you consider when generating a figure that contains chemical structures? How do you decide how to represent the chemical/residue structure(s) (i.e., level of detail, color, mechanisms, etc.)? What program(s) do you prefer for generating such figures and why? The scientists we hear from in this installment are Ruma Banerjee, primary author of 'Gas regulation of complex II reversal via electron shunting to fumarate in the mammalian ETC' ([1], see Figure 2) and Yael David, primary author of 'Non-enzymatic covalent modifications as a new chapter in the histone code' ([2], see, e.g., Figure 3), and Jennifer C. Chan, first author of 'Nothing is yet set in (hi)stone: novel post-translational modifications regulating chromatin function' ([3], see Figure 2).

Zen and the art of science illustration

In *Fathers and sons*, the protagonist, a student of medicine, notes wryly that a 'drawing shows me at one glance, what might be spread over ten pages in a book'. Despite the irony that this nod to brevity appears in an 1862 work of prose by Ivan Turgenev, it highlights the importance of art as an effective medium for science communication. In science, where it is essential that the data does the talking, placing a premium on high-quality illustrations is key to animating the conversation. Here, I focus on three general considerations for generating aesthetically pleasing and informative figures: the use of consistent font style and line thickness, the judicious use of color, and effective labeling.

While the choice of font and display options might seem too mundane to merit discussion, they are in fact foundational to tidiness, presentation quality, and legibility, following reduction upon typesetting. Figures can be drawn or assembled with a variety of software (e.g., Adobe Illustrator and Microsoft PowerPoint), while ChemDraw (with the Helvetica font) is particularly well suited for chemical structures. A favorite refrain that color should

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be used to convey information implies that if colors are employed to differentiate between species (e.g., redox states in metalloproteins), then use of the same colors to denote corresponding properties (e.g., spectra) increases accessibility to the information. Which leads me to the final point: the value of clear labeling to facilitate data interpretation independent of the details provided in the legend. Embracing the Zen design principles of simplicity and completeness for communicating in ‘one glance’ is ever more germane as the publication tsunami challenges attention span.

Designing engaging figures: enhancing communication at the chemical biology interface

Working at the interface of chemistry and biology, we aim to provide details at a level that will appeal and be comprehensive to both communities. In our efforts to enhance scientific communication, we recognize the importance of figure design and color choices in conveying information effectively. In our recent *Trends in Biochemical Sciences* article, we employed a thoughtful approach to generate figures that facilitate understanding and engagement.

To create visually compelling figures, we predominantly utilized a combination of BioRender and ChemDraw. BioRender served as the preferred tool for non-chemical structures, while ChemDraw was employed for generating chemical structures. This combination allowed us to leverage the unique capabilities of each software, optimizing the representation of diverse molecular components at the interface between chemistry and biology. The structures were merged using BioRender and Microsoft PowerPoint. The seamless integration of chemical and non-chemical elements was a key aspect of figure design, ensuring a cohesive depiction of complex biological and chemical interactions.

In selecting colors for residues, our approach focused on highlighting regions of change or activity within the molecules. This strategic color coding aimed to draw attention to the relevant features, enabling readers to quickly identify and comprehend key aspects of the figure. By employing this technique, we sought to enhance the visual clarity and aid the interpretation of the depicted molecular mechanisms.

Furthermore, our color choices were driven by the objective of providing strong visual contrast without overpowering the accompanying text. We aimed to strike a balance between making figures visually appealing and ensuring that they seamlessly integrate with the overall scientific narrative. The intention was to create figures that are visually striking yet do not detract from the essential information presented in the article.

In summary, we broadly aim to leverage figure design and color choices to emphasize our message. By utilizing a combination of BioRender and ChemDraw, we have integrated chemical and non-chemical structures to create coherent representations. Our color choices aim to enhance visual contrast and draw attention to important molecular features, while ensuring that they complement the accompanying text. Through these practices, we strive to deliver figures that effectively communicate complex concepts to a broad audience of scientists at the chemistry–biology interface.

Painting a picture worth a thousand discoveries

What is the main message of your figure? To create an effective figure, it's important to have a clear objective in mind. One approach is to determine the title before starting the design process. For instance, in our review, we wanted to illustrate the advancements in novel histone post-translational modification (PTM) discovery. Once the objective is established, you can then begin focusing on the content. Figures should be used to highlight key points from your manuscript without overwhelming the reader with excessive information. Striking a balance between being informative vs. overloading is important to prevent confusion. In our schematic, we wanted to convey a lot of information about chemical structures, location, and regulation of several histone PTMs. To enhance the clarity of these complex ideas, we employed elements of visual design.

Colors, preferably from a colorblind-friendly palette, and spacing are great strategies for visually organizing themes. Colors can group related concepts or signify distinct ideas. By playing with opacity and brightness, colors can highlight focal points or downplay unessential elements. When it comes to chemical structures, consider the level of detail required. Lewis structures can make figures appear cluttered, so if your message can be conveyed using line structures, it will help simplify the figure. Additionally, take advantage of common symbols that don't require additional explanation. By incorporating equilibrium arrows, we were able to succinctly present each PTM with their precursors and regulators. We also used images to indicate the physiological relevance of each PTM. Not only does this provide additional information, but it visually helps direct the reader's eye to focus on each PTM individually. Finally, consider whether someone would use your figure in a talk. Keeping this in mind will help ensure that your figure is clear, informative, and visually appealing.

Biographies

Ruma Banerjee

Yael David

Jennifer C. Chan

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