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Coloring Chemistry—How Mindful Color Choices Improve Chemical Communication

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Abstract: *Color is a central element to scientific communication, but its use comes with the responsibility to ensure universally accessible and accurate data presentation. This short Viewpoint Article aims to sensitize the chemical community to the importance of mindful color choices in scientific illustrations.*

Chemical communication on all levels relies on the accurate depiction of structures, transformations, and data in figures, schemes, or combinations thereof: Chemistry is a visual science. In this context, color can be a powerful tool to highlight elements of a figure, guide the reader's eye, or convey information. Colors are often easier to perceive and differentiate than shapes and can be particularly helpful to enhance recognition of recurring elements or intuitively link to concepts. However, improper color choices can lead to a misrepresentation or inaccessibility of the underlying information.[1] Indeed, a survey of several recent issues of prominent chemistry journals showed that more than two-thirds of their articles contain colored figures in their main text whose information content is not accessible to people with color vision deficiencies.[2] This prevalence of inaccessible visual representations of data and conclusions stands in stark contrast to the spirit of inclusive and open science. Therefore, we herein aim to raise awareness to the importance of mindful color choices in chemical communication and formulate guiding principles to ensure a faithful and inclusive representation of information in scientific illustrations.

Color can serve a variety of purposes and it is important to differentiate between color as a supporting element and color as an information-coding element. As a supporting element, color is intended to enhance a figure's visual appeal or highlight certain parts of a graph or scheme. Here, the choice of color is unproblematic and may be decided by personal preference. This additional layer of information introduced by color solely aims to guide the reader's eye and does not represent data. Thus, a potential loss of this layer does not diminish the overall message and information content of a figure, which grants the artist almost unlimited freedom in terms of color choices. In contrast, color choices are crucial once color serves as an information carrier. Color-coding of information inherently requires readers to recognize and differentiate between the colors used, which can be challenging or impossible for people with color vision deficiencies (ca. 4% of the total population).[3]

This holds particularly true for the color combinations involving red, blue, black, and green, which seem to be ubiquitous across the chemical literature,[4] most likely because they appear among the default color choices of many popular scientific data processing programs.[5,6] The main problem with this particular color combination, and also many others, is the lack of visual difference between at least two of these colors for people with reduced color perception.[7] This can make the information content of a figure partially or completely inaccessible when colors in the legend or colors of structural drawings appear identical (Figure 1A). While complete color-blindness is rare, reduced sensitivities of red (protanomaly) or green retinal receptors (deuteranomaly) are relatively common. Thus, there exists a particular bias for misrepresentation and/or loss of information in figures containing combinations of red and green or different hues thereof (see Figure 2 for a case study). In addition, having multiple colors of similar luminosity in a figure introduces a burden for readers who print an article in grayscale, as this reduces the three-dimensional RGB color space (trichromatic space) to a one-dimensional spectrum of lightness/darkness (monochromatic space). Colors which could be recognized with ease in a three-dimensional color space can become impossible to discriminate by luminosity alone, making the underlying information inaccessible. Therefore, we recommend designing illustrations in a fashion that uncouples color recognition from data accessibility: Color recognition should be optional to access a figure's information content.

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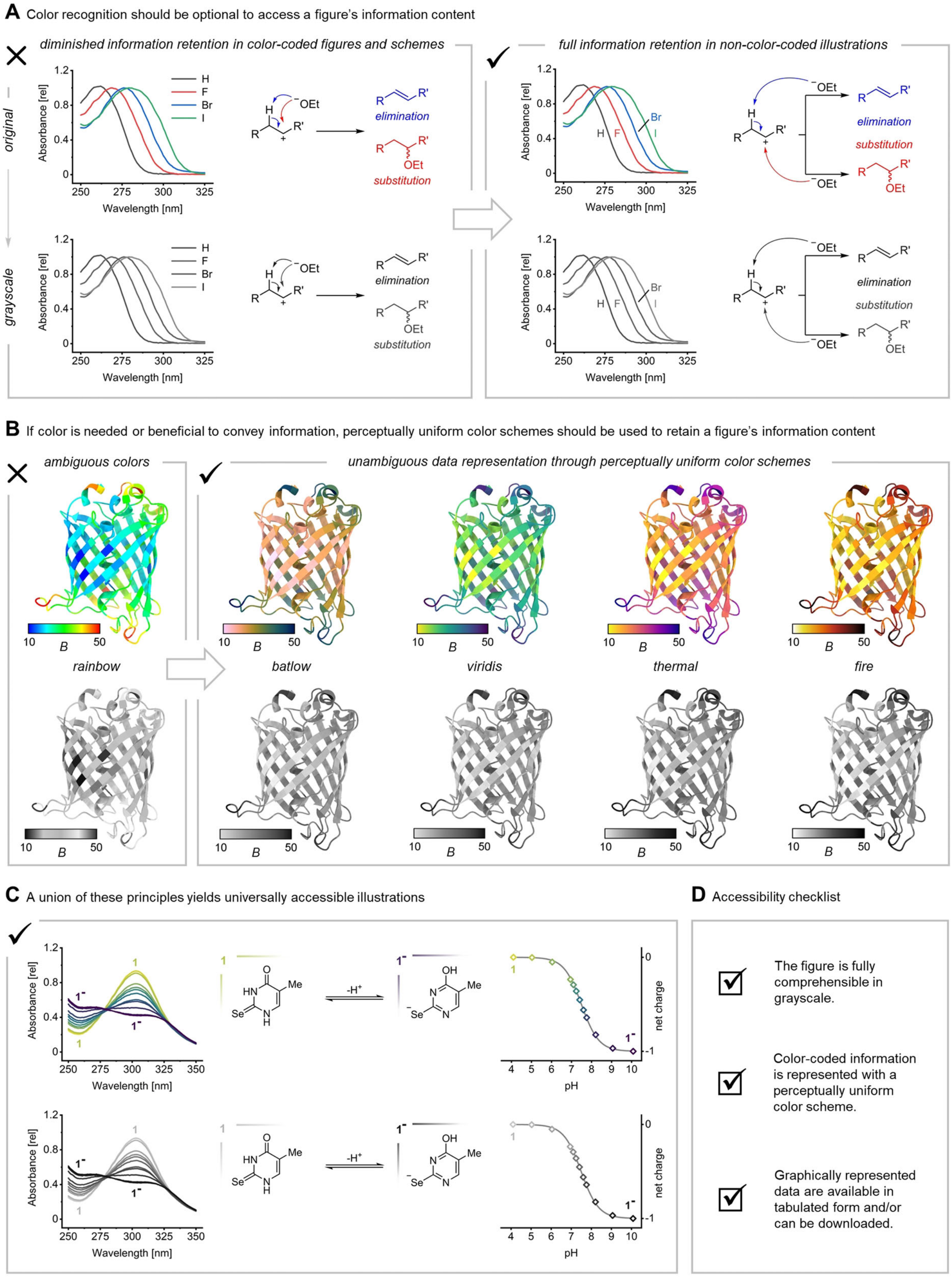

Figure 1. Color choices impact a figure's accessibility, as the retention of information during color reduction hinges on the role color plays as well as the color combinations used. The graph in (A) represents UV absorption spectra of a halide series of uridine analogs (taken from ref. [10] and available online at ref. [11]). For the coloration of the graph and the structural drawing, the default colors of Origin 2020b and ChemDraw 16 were used. (B) displays B-factors (*B*) of a GFP variant (PDB ID 5b61) as assessed with UCSF ChimeraX 1.2.5 in various openly available color schemes like batlow from ref. [1] (available online at ref. [12]). (C) shows the pH-dependent UV absorption properties of a selenopyrimidine (**1**), reflecting its pK_a value (data taken from ref. [13] and available online at ref. [14]), and illustrating the principles summarized in (D).

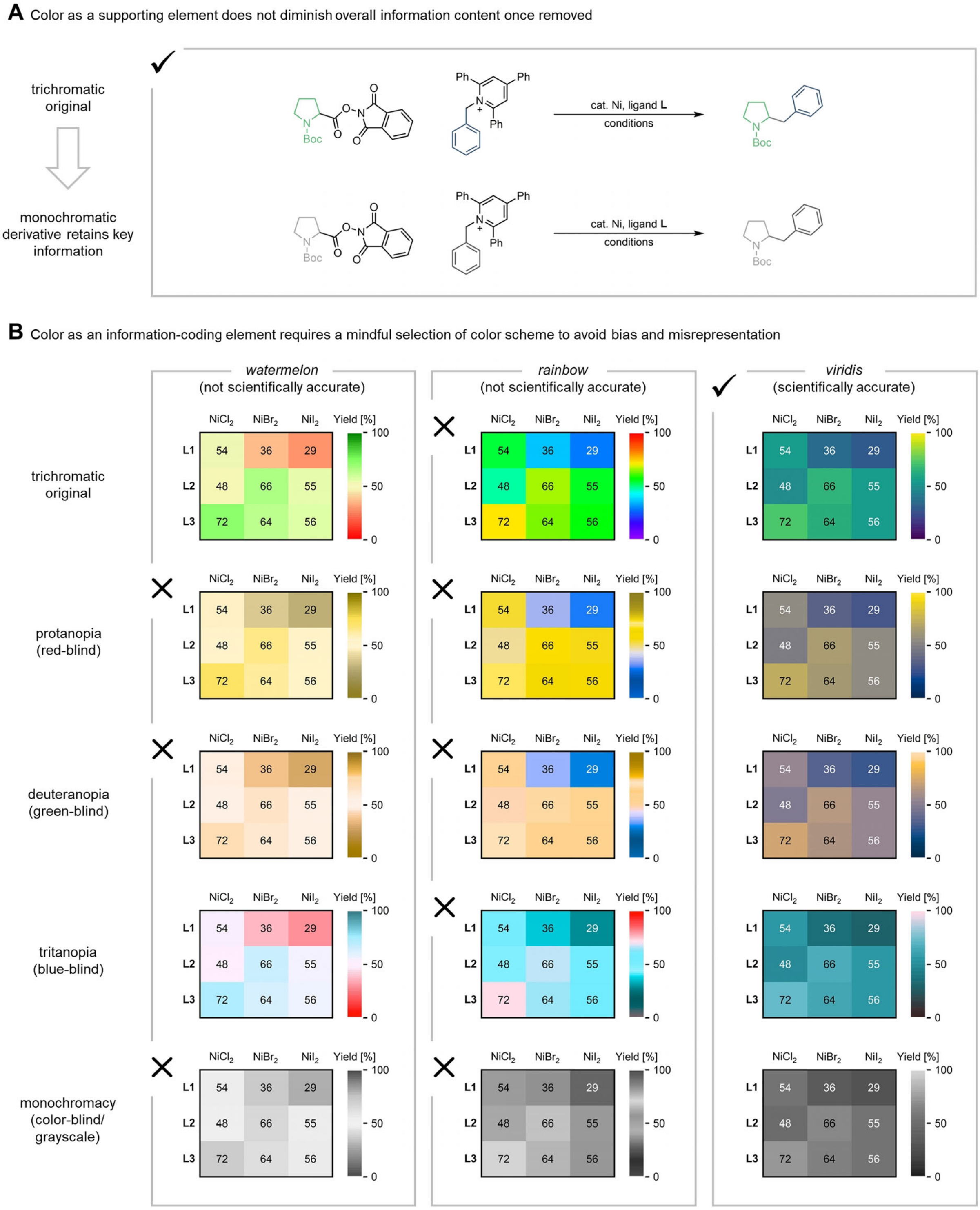

Figure 2. The function of color in an illustration determines the necessary attention to detail. A) As a supporting element, color does not transmit key information and colors may be chosen based on any personal preference. A reduction of the three-dimensional (trichromatic) color space to a one-dimensional (monochromatic) one fully retains the key information content of the figure. B) As an information-coding element, color conveys quantitative information, which necessitates the selection of a scientifically accurate color scheme to avoid the introduction of artifacts and biases. For instance, the optimization data for the reaction shown in (A) are accessibly and fairly represented by a viridis color map (as used by Zhang and Cernak in the original publication),[15] while a watermelon or rainbow scheme is not universally readable, perceptually uniform or ordered. The data shown in (B) are a subset of data from a 24-well screen taken from Zhang and Cernak's[15] Supporting Information (displayed in their Figure S22 and available for download at ref. [16]), where **L1** = [2,2′-bipyridine]-5,5′-dicarboxylic acid, **L2** = dimethyl [2,2′-bipyridine]-5,5′-dicarboxylate, and **L3** = 4,4′-bis(trifluoromethyl)-2,2′-bipyridine.

Although many figures can be designed to bypass the need for color recognition, there are instances in which the representation of data as color is of great benefit or even necessary. For instance, multidimensional data often benefit from a condensed description in heatmaps, contour plots, or structural drawings.[8] However, this color-coding requires a mindful choice of colors to avoid misrepresentation and loss of information.[9] The same problems encountered with combinations of red, blue, black, and green carry over to the popular rainbow (also known as jet) color map. This color scheme, and others, often create perceptual ambiguities due to a non-uniform and non-linear gradient of lightness and saturation along the map (also see ref. [1] and references therein). Thus, rainbow-colored illustrations typically exhibit artificial gradients and contrasts that are not reflected by the underlying data or hide real details of the data. This is especially troubling in cases where the underlying data are not published along with the figure, because it inevitably leads to a loss of information even when the figure can be viewed as intended. To resolve this issue, we recommend the consistent use of perceptually uniform color schemes (also known as scientific color maps),[1] which retain color-coded information content for all readers (Figures 1 B and 2 B).

In contrast to the popular rainbow color map, scientific color schemes have four key characteristics, which advocate for their use across the scientific literature. First, *perceptual uniformity* provides an equal weighing of data across the displayed data space. Thus, a given variation of the data results in a given color (or lightness) variation, regardless of where in the data space this variation occurs. Secondly, *perceptual order* ensures that all individual colors in a map can be ordered sequentially without consultation of the color bar. This significantly enhances the intuitive understanding of the parameter space as well as the underlying trends. Such an order can be created by assigning a monotonic change in hue from one color to another, or lightness between light and dark colors, or both. Thirdly, *universal readability* establishes that a figure can be understood by all readers. To this end, color maps require a monotonic lightness gradient, maintaining the full information content even when parts (color vision deficiency) or all (color-blindness) of the multidimensional color space is removed from a figure. Generally, examination of a figure in grayscale serves as a good bench test for these first three principles. Lastly, *instinctive readability* makes the information content of an illustration as understandable as possible by providing intuitive coloring. This can be achieved by using colors that reflect and relate to the nature of the depicted parameter, or its high and low values (for instance by having red relate to hot temperatures or having black relate to empty space or no yield).

Given these prerequisites for scientific color maps, it is easy to recognize why most color schemes may be less than ideal. However, extensive research on human color perception and inclusive data representation has afforded guiding principles for scientific color choices[17–21] as well as a diverse set of scientifically accurate color schemes. Many of these schemes are freely available for download (e.g. at ref. [12]) and popular choices include the viridis, thermal (or its variants plasma and magma), and fire (also known as kry) schemes (Figure 1 B). Other common options include the cividis color map, which was designed to look identical through the lens of all types of color vision deficiencies, and batlow, which offers a broader range of distinctly recognizable colors than its peers. Considering the immense heterogeneity and different types of data that authors across the chemical sciences may wish to display, it is impossible to assign a "best" scientific color map, or one that fits every purpose. Therefore, it is best to consult several different options for a given dataset to identify the most suitable color scheme (a flowchart for color map selections is also described in ref. [1] and available at ref. [22]). Since many parameters offer themselves to representation with several different color maps, the available variety of scientific color maps also grants quite some artistic freedom to authors. It should also be mentioned that scientific color maps are useful tools for purposes beyond accurate color-coding of information. Their inherent perceptual order and instinctive readability also make them remarkably effective as supporting elements for figures which do not strictly require them (for instance viridis in Figures 1 C and 2 A).

In conclusion, we believe that a union of the principles outlined above yields universally accessible illustrations, utilizing color to guide its viewers, while retaining their full information content even when reduced in color (Figure 1 C). To implement these principles in the chemical literature, we appeal to all authors, reviewers, and editors to consider a figure's information accessibility during the writing or publication of a paper. An ideal figure should 1) be fully comprehensible once reduced in color content, 2) represent color-coded information with a scientifically accurate color map, free from artificial gradients and color ambiguity (e.g. the ones listed in ref. [1]), and 3) be accompanied by the underlying data in tabulated and/or downloadable form (Figure 1 D). Ultimately, scientific illustrations should be accessible to everyone. However, to realize this cornerstone of open and inclusive science, visual sciences like chemistry require a reflected design of figures. We hope that this short Viewpoint Article will serve as a resource to communicate and raise awareness of the issue of mindful color choices among colleagues, departments, and institutions, since a true improvement of the accessibility of illustrations in the chemical literature is, and will remain, a community effort.

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Conflict of Interest

The authors declare no conflict of interest.

Disclamer

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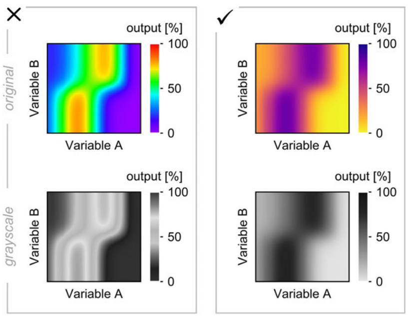

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