The purpose of this tutorial is to help you understand the relationship between conjugated molecules and their color (if there is any). Let us begin!

First, a quick definition of conjugation:

**Conjugation:** special stability gained by the overlap of 3 or more p orbitals. This can be achieved via pi-sigma-pi bonds or can be achieved by an atom (like nitrogen or oxygen) with a lone pair that is sp² or sp hybridized.

Second, how does our eye perceive color?

We see an object – or molecule – as colored when the object absorbs light at a wavelength that matches some wavelength in the visible light spectrum (about 400-700 nanometers). If a molecule absorbs orange light, we say the molecule is blue. This conclusion is based on complementary colors: Find the color that the molecule absorbs and then look directly across it (follow the arrow) to find what color we would see it as.

So how do these two seemingly unrelated ideas relate?

Highly conjugated molecules can be colored.

Okay...this is not to say that ALL highly conjugated molecules ARE colored or that all unconjugated molecules are NOT colored. There are many other factors that can
affect a molecule’s color (i.e. many transition metals are colored, NOT due to conjugation).

When a molecule absorbs a photon of some energy, one electron moves up to a higher energy orbital. Now, there is a gap between that one electron in the higher energy state and the electron in the lower energy state, we call this the HOMO/LUMO gap or $\Delta E$.

This value, $\Delta E$, may correspond to an energy that is absorbed by a photon in the visible light spectrum (shown below). If this occurs, the molecule will be colored. What color you will see is dependent on what wavelength the HOMO/LUMO gap refers to. If it corresponds to 700 nanometers, you would see a green molecule (see complementary colors).

From the image above, we can see that lowest wavelengths absorb violet (so we will see yellow) and the highest wavelengths absorb red (so we will see green).

This means that molecules with a low HOMO/LUMO gap may be yellow and molecules with a high HOMO/LUMO gap may be green.

Going back to what we said earlier, highly conjugated molecules can be colored.

Example: Is 1,3-pentadiene colored?

Probably not, because it is not highly conjugated.
Example: Is this molecule colored?

Probably. In fact, the above compound is the Heme group of hemoglobin, which gives blood its red color. So, it would absorb photons that correspond to green light (about 600 nm) so that we see red.

We can only make assumptions about what color a molecule might be if we know what color a SIMILAR molecule is. If the molecular structures differ significantly (for example, differing functional groups, different number of conjugated atoms, different atoms entirely), we cannot make ANY assumptions on what color a molecule is.

Example:

Given that retinol is yellow:
What color do you expect retinal to be?

A reasonable guess would be orange because it is more conjugated, so its HOMO/LUMO gap would be less than retinol’s. Its energy would be lower, so it’s wavelength, often denoted by $\lambda$, would be higher. Retinol absorbs purple light, corresponding to about 400nm. Retinal absorbs blue light corresponding to about 450nm.

As the HOMO/LUMO energy gap decreases, the wavelength of the absorbed color increases. To find the perceived color, look back at the complementary colors image above.

This can be explained by the equation:

\[ E = \frac{hc}{\lambda} \]

Energy and wavelength have an inverse relationship. As the energy difference goes up (i.e. less conjugated) the wavelength decreases, spilling into the UV region, giving us a colorless molecule. As the energy difference goes down (and conjugation goes UP) the wavelength increases, spilling over into the infrared region.
Works Cited


Images:

Complementary color image:
http://www.sapdesignguild.org/goodies/glossary_color/IMAGES/trad_comp.jpg

Visible light spectrum image:

Retinal image:
https://upload.wikimedia.org/wikipedia/commons/thumb/1/1b/11-cis-Retinal.svg/354px-11-cis-Retinal.svg.png

Retinol image:
http://pangansehati.files.wordpress.com/2009/10/800px-retinol-svg.png

1,3-pentadiene image:
http://upload.wikimedia.org/wikipedia/commons/thumb/2/28/1,3-pentadiene_(hydrogens).svg/120px-1,3-pentadiene_(hydrogens).svg.png

Heme image:
http://upload.wikimedia.org/wikipedia/commons/thumb/b/be/Heme_b.svg/200px-Heme_b.svg.png