Color of substances

Many substances contain a valence electron that can be excited to a higher energy level by electromagnetic radiation. Such a substance then absorbs radiation of a certain wavelength with an energy photon corresponding to the energy difference of the two electron levels. If the absorbed radiation lies in the visible part of the spectrum, the substance will appear coloured to the human eye (it will have a colour complementary to the colour of the absorbed light).

Absorbed wavelength (nm)		Matching colour	Complementary colour	
380–435		purple	yellow-green	
435–480		blue	yellow	
480–490		green-blue	orange	
490–500		blue-green	red	
500–560		green	purple	
560–580		yellow-green	purple	
580–595		yellow	blue	
595–650		orange	green-blue	
650–760		red	blue-green	

Unfortunately, it is not easy to predict the colour of a substance on the basis of its chemical structure, nor is it possible to infer the composition of a substance unambiguously from the absorption spectrum. However, from our point of view, three groups of substances that are often coloured are relevant:

1. Substances containing a system of **conjugated double bonds** whose molecule is not symmetrical. If we imagine a symmetric conjugated double bond system, it can exist in two resonance states that are energetically equivalent: The presence of an asymmetric substituent will cause the energies of the two states to be different. The energy difference often corresponds to the energy of a photon in the visible part of the spectrum. Typical representatives may be dyes with a polymethine chain (–CH=CH–CH=CH–) nor azo (-N=N-). Substances with aromatic or heterocyclic structures bonded to a common central atom (e.g. triphenylmethane dyes) behave similarly.
2. Also, the d and f valence electrons often determine the color of the compound. They tend to be present in coordination covalent bonds complex compounds. For example, anhydrous copper sulfate $CuSO_4$ is colorless, while its pentahydrate $CuSO_4 \bullet 5H_2O$ and its aqueous solution are blue: in both cases, because copper enters a complex with water $[Cu(H_2O)_4]^{2+}$. In a similar way, colored and complex compounds of other transition metals (Fe, Cu, Cr, Mn, Ni, Co) tend to be complex-bound metal also in the colored proteins of hemoglobin and cytochromes.
3. Ions containing a transition metal with a **high oxidation number** as the central atom are also coloured, e.g. MnO_4^-, $Cr_2O_7^{2-}$.

Analytical methods used in medicinal chemistry and biochemistry make use of all three groups of colored compounds. Systems of conjugated double bonds are often formed in reactions in which the analyte condenses with a suitable chromogen (e.g. creatinine with picric acid in the Jaffé reaction, diazo-coupling reactions in the detection of bilirubinu), or are formed by oxidation of a chromogen that contains one double bond less (oxidation of benzidine derivatives in peroxidase reactions). The formation of colored complexes is used, for example, in the determination of proteins by the so-called biuret reaction (Cu^{2+} complexes with O and N peptide bonds) or in the detection of a number of substances, e.g. with $FeCl_3$. Color changes during the reduction of Cr^{6+} to Cr^{3+} are used, for example, in the detection of ethanol in exhaled air.

Absorption of monochromatic light can also be conditioned by events other than electron excitation. These are primarily changes in the various oscillation energies of atoms in molecules and the rotational energies of entire molecules. These principles are used more in fluorimetry. From the point of view of medical biochemistry, they are much less important than the above principles.