1-Spectroscopy: Interaction EMR-Matter

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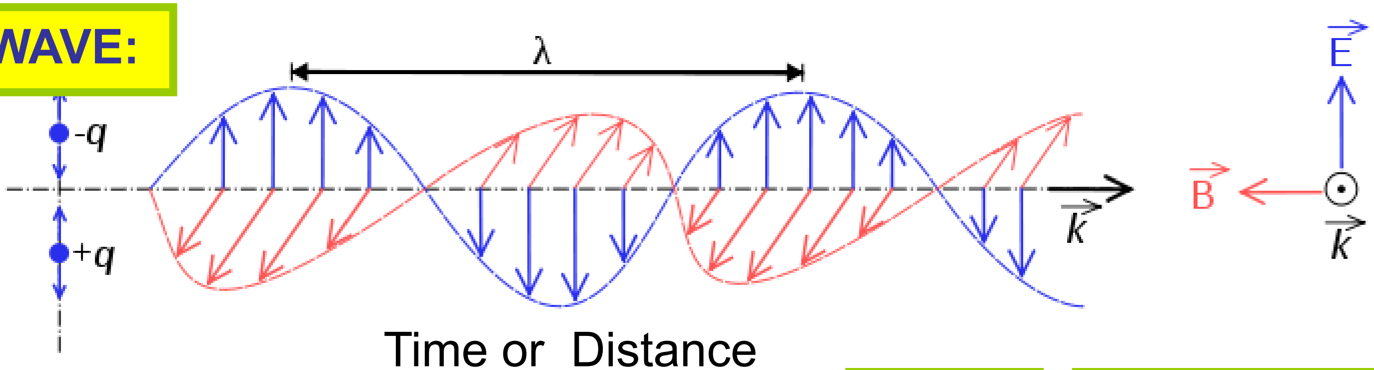
1. PROPERTIES OF ELECTROMAGNETIC RADIATION

- **WAVE – PARTICLE DUALITY**

1- WAVE:



– ν: ***Frequency***: number of oscillations per time unit **$\nu = 1/T$** **UNITS: s^{-1}**

– λ: ***wavelength***: distance between two equivalent points in the wave, maxima or minima, consecutive

UNITS: inverse of length: Å, nm, cm, m...

– $\bar{\nu}$: ***Wavenumber***: **$\bar{\nu} = 1/\lambda$** **UNITS: length: $Å^{-1}$, nm^{-1}, cm^{-1}, m^{-1}...**

v: ***Speed***: **$v_i = \nu \lambda_i$** **UNITS: m/s** **c**: ***vacuum speed*** = 2,99792 x 10^8 m/s **(≈air speed)**

2- PARTICLE:

PHOTONS: Energy: $E = h\nu$

UNITS: Jules, electron volt

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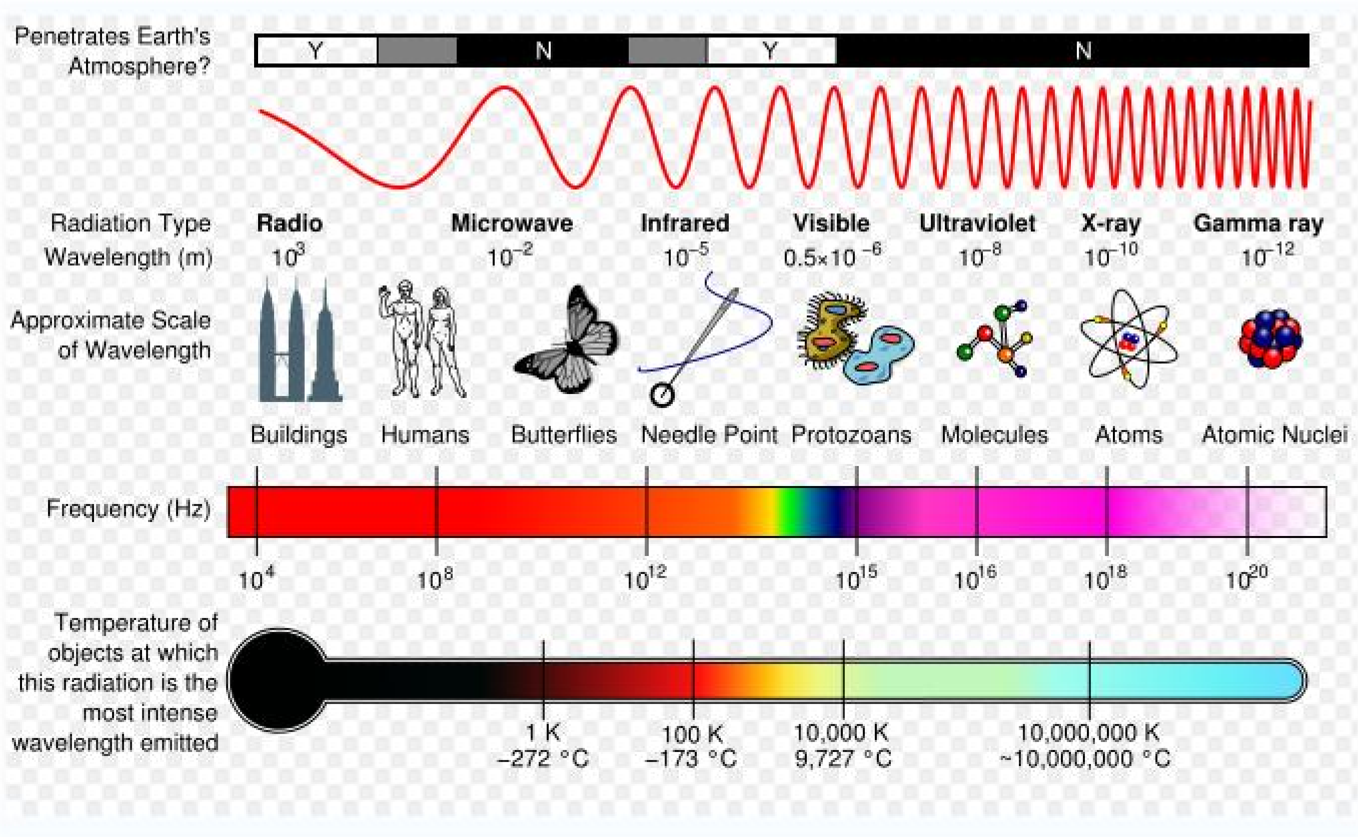
ELECTROMAGNETIC SPECTRUM



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2- PROPERTIES OF MATTER

ENERGETIC LEVELS OF THE MATTER

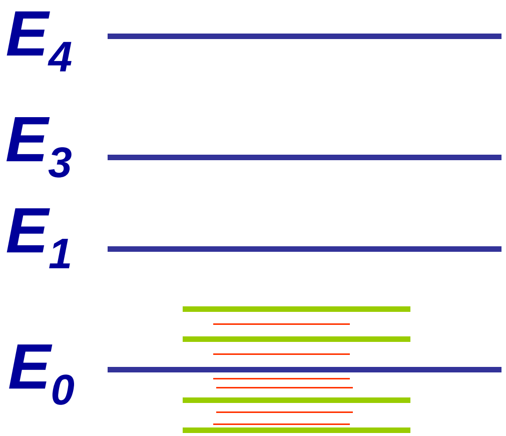
$$E = E_{traslational} + E_{rotational} + E_{vibrational} + E_{electronic} + E_{nuclear}$$

MW

IR
RAMAN

UV-VIS
R-X

$$E_{rotational} < E_{vibrational} < E_{electronic}$$



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3- ELECTROMAGNETIC RADIATION-MATTER INTERACTION

TRANSITIONS BETWEEN ENERGETIC LEVELS OF THE MATTER

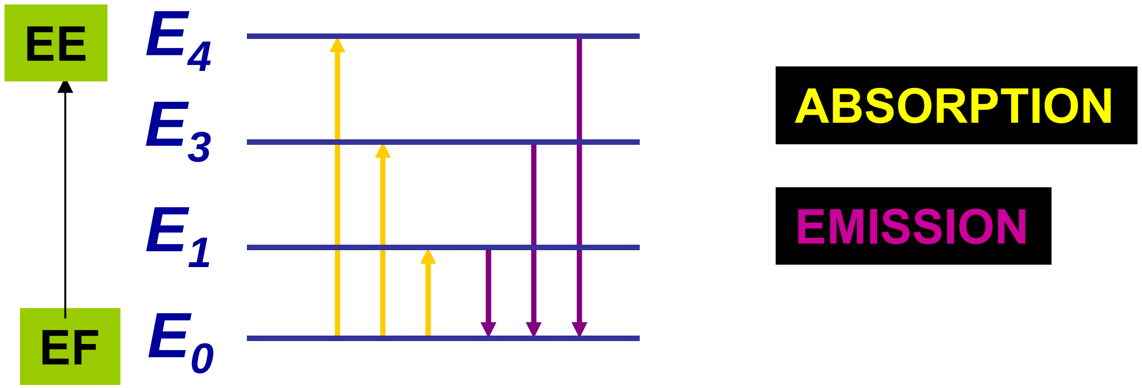
• **QUANTUM THEORY :** Max Planck (1900)

1- Matter (atom, ion or molecule) wins or release EXACTLY the amount of energy that separates two energetic levels of the matter.

2- BÖHR´S CONDITION: Electromagnetic Light: should be EXACTLY of the same energy that separates two energetic levels of the matter.

4- TYPES OF SPECTRA

- $E_1 - E_0 = h\nu = hc/\lambda$
- $E_1 - E_0 = h\nu = n\,(h\nu/n)$ h= 6,62617610^{-34}Js



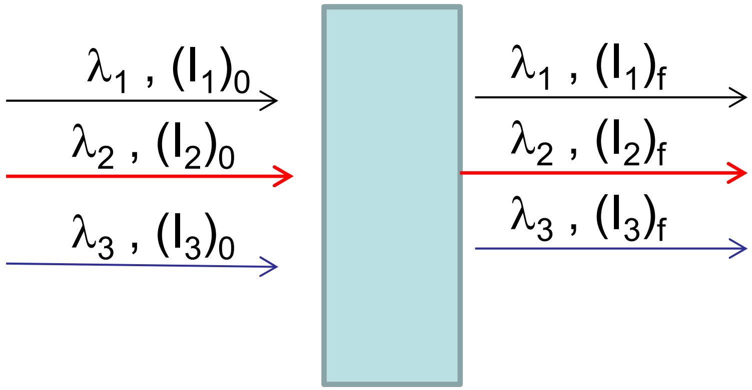
- T_{ROOM}: FS

ENERGY AND SEPARATION OF THE LEVELS DEPEND ON:
- CHEMICAL STRUCTURE OF THE MATTER
- INTERACTION WITH OTHER MOLECULES: SOLVENT OR SOLUTES

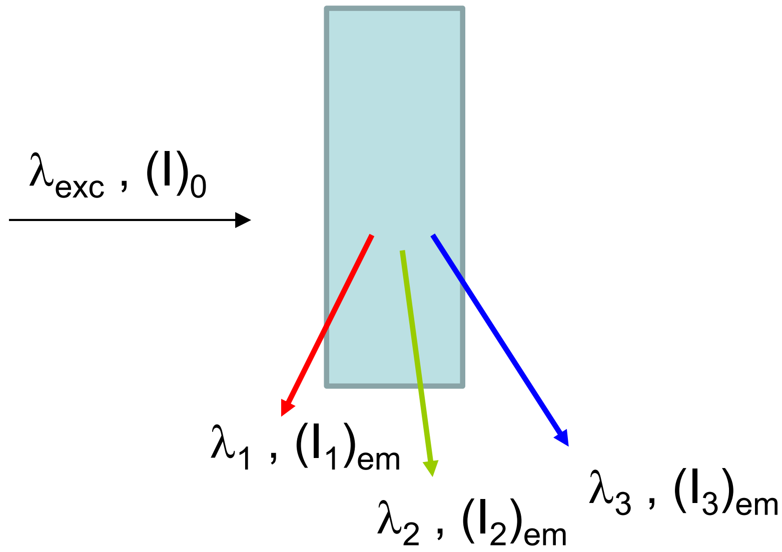
5. ABSORPTION AND EMISSION SPECTRA

SPECTRUM: INTENSITY OF LIGHT vs WAVELENTH

ABSORPTION



EMISSION



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6. WHAT IS NEEDED FOR GETTIN ABSORPTION AND EMISSION SPECTRUM?

ABSORPTION

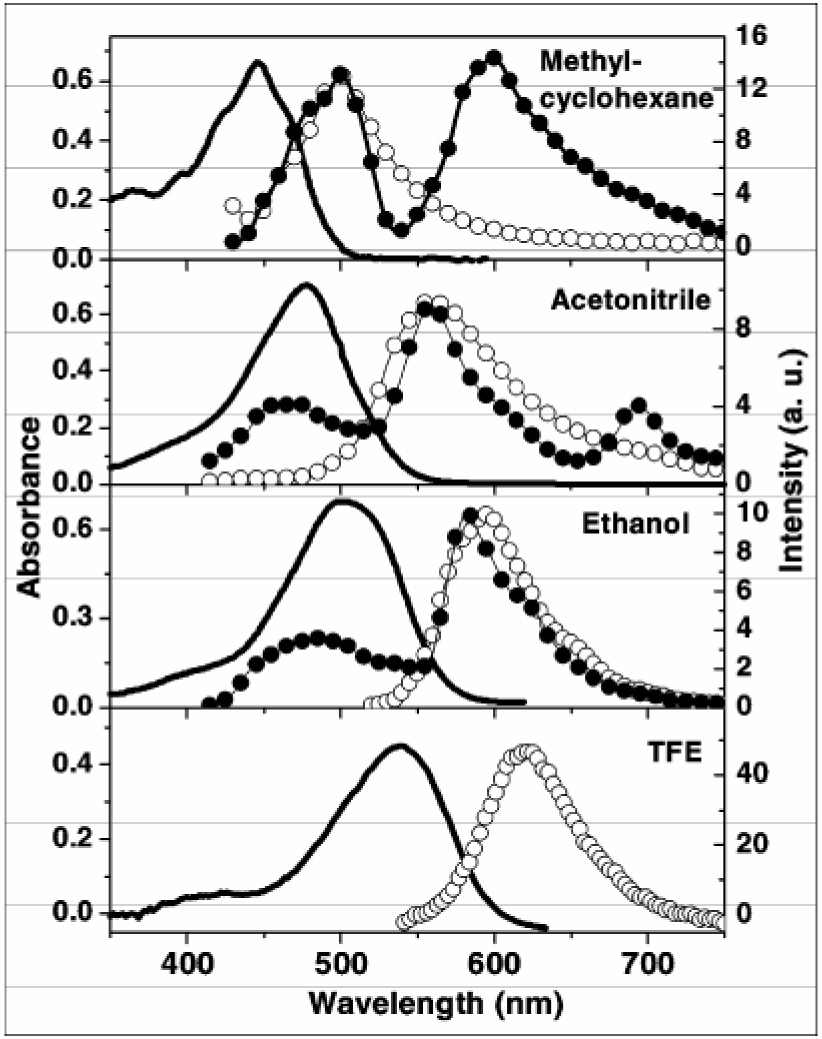
- 2º: *The Wavelength Range Where Compound Absorbs*

EMISSION

- 1º: *Sample Excitation With An Adequate Wavelength: Absorption Spectrum*

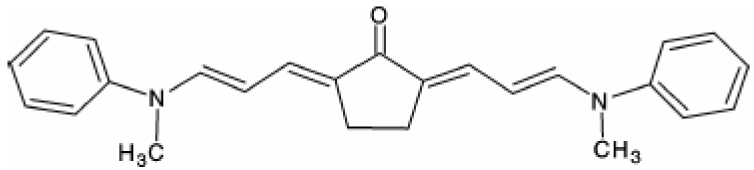
- 2º: *Measure The Emission In The Wavelength Range Where Compound Emits:* $\lambda em > \lambda exc$

7. ABSORPTION AND EMISSION SPECTRA OF NATURAL PRODUCTS



KETOCYANINE

Ground-state absorption spectra (solid black line) and fluorescence spectra of MPAC recorded in different solvents using 400 nm photoexcitation at room temperature (open circles) and in solid matrices at 77 K (solid circles).



Scheme 1. Chemical Structure of MPAC.

J. A. Mondal, S. Verma, H.N. Ghosh and D. K. Palit, *J. Chem. Sci.*, Vol. 120, No. 1, January 2008, pp. 45–55

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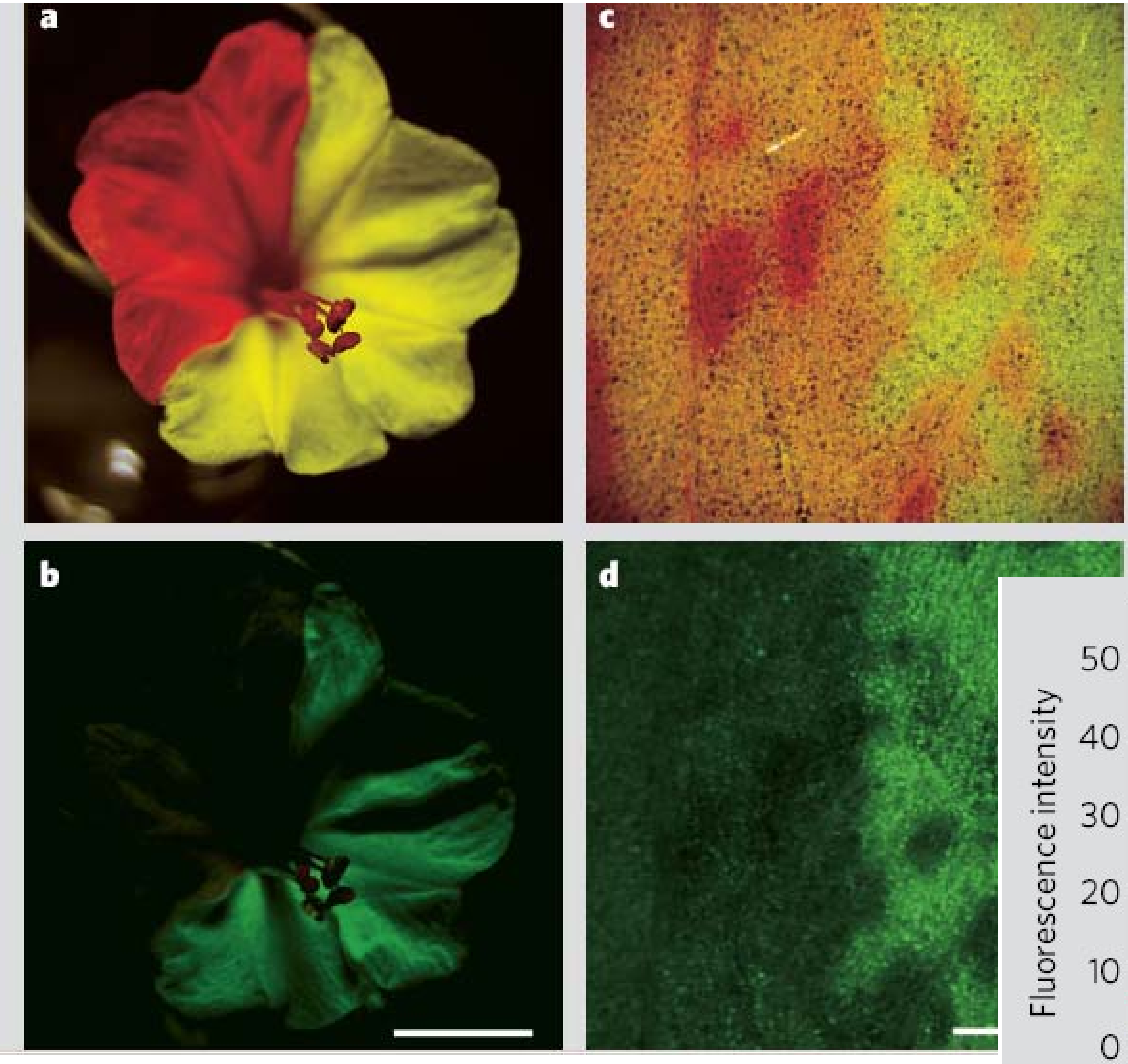
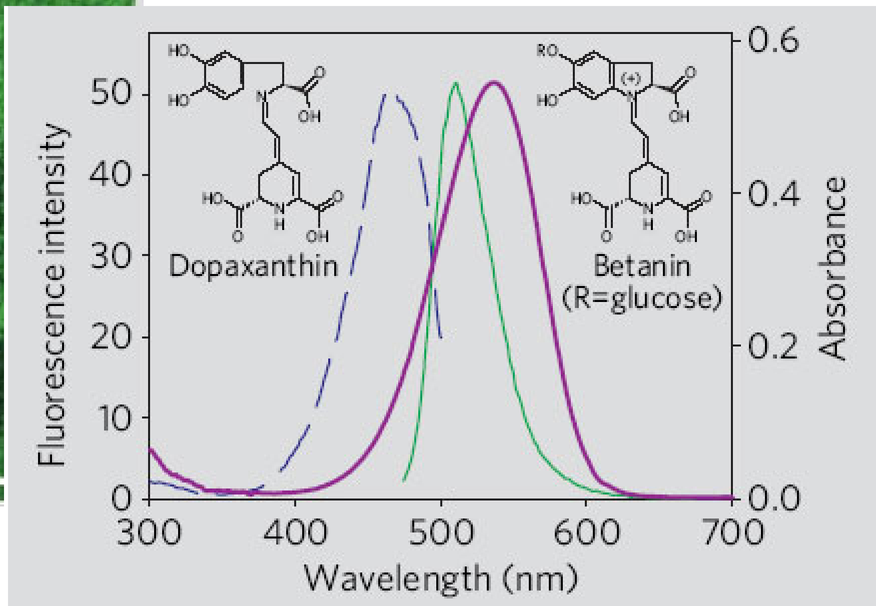
Fernando Gandía-Herrero[1], Francisco García-Carmona[1] & Josefa Escribano[1], *Nature*, **437**, 334, 2005.|doi:10.1038/437334a;

Visible fluorescence in *Mirabilis jalapa* petals.



a, b, Flower with areas of red or yellow coloration under white light (**a**); only the yellow areas emit green fluorescence when excited by blue light (**b**) (scale bar, 1.5 cm). **c, d,** Light micrographs of a section of a single red-and-yellow petal, showing brightfield (**c**) and fluorescent (**d**; excitation wavelength, 450–490 nm) images (scale bar, 500 m). Green fluorescence is due to betaxanthins; dark areas correspond to orange areas in **c**, where light emitted from the fluorescent pigment is absorbed by betanin.



Excitation (Blue) and emission (Green) spectra of Dopaxanthin
Violet: absorption espectrum of natural betanin

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Absorption and Emission Spectra of Chlorophylls a and b

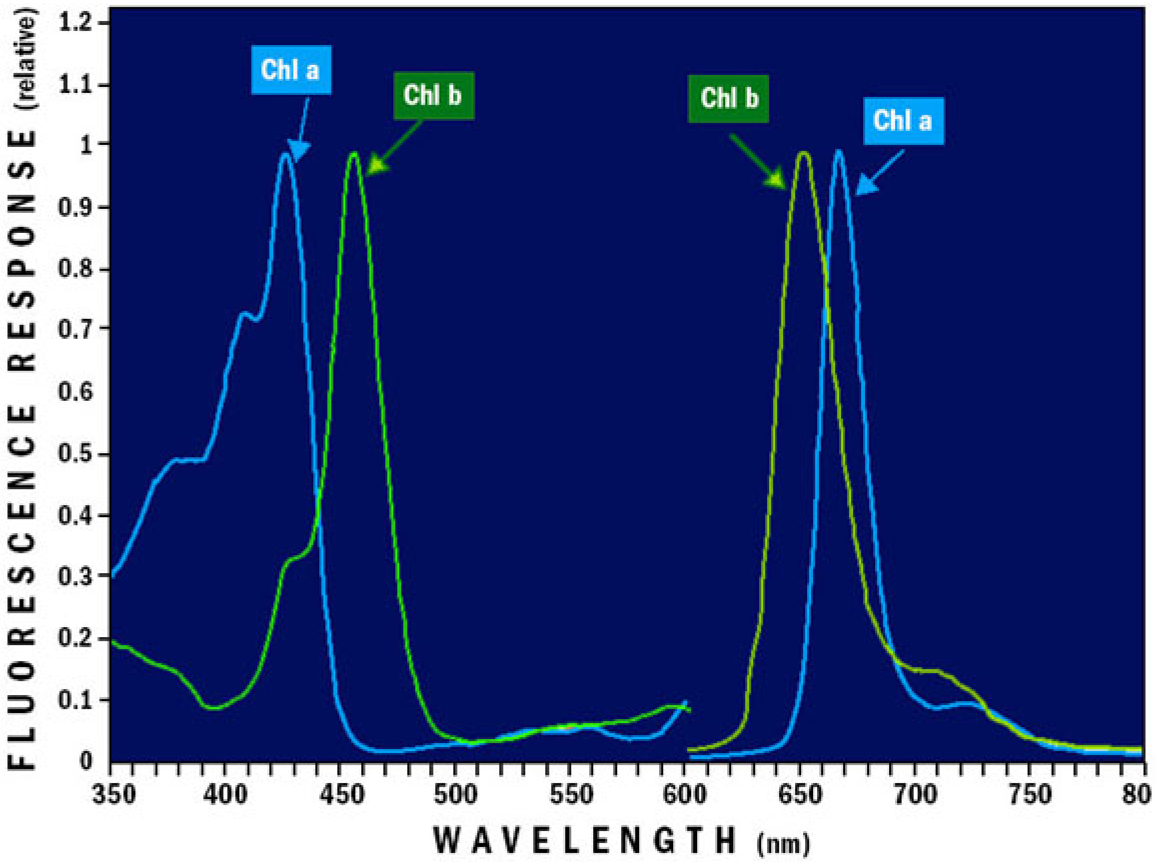
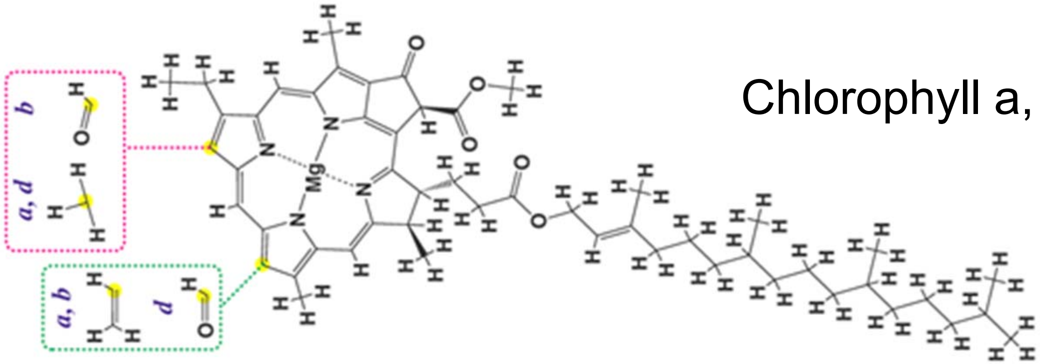


Figure 3: the excitation and emission spectra for chlorophyll-a and chlorophyll-b. The excitation spectra are on the left and the emission spectra are on the right. Say you wanted to excite fluorescence in chlorophyll-a as much as possible. Then you'd want to excite it with light having a frequency at the peak of its excitation spectra: somewhere around 425 NM If you did this, the light given off would have the spectral distribution as shown, being peaked around 680 NM If you had a mixture of Chl-a and Chl-b and wanted to primarily excite the Chl-b, you might choose to excite the sample at around 470 NM because the Chl-a excitation spectrum is very small while the Chl-b is very big, meaning that the Chl-a wouldn't fluoresce much but the Chl-b would.



Chlorophyll a, b and d chemical structure

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EMISSION

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8. REMEMBER

* The absorption and emission spectra are alike, since the levels involved are the same

* BUT the wavelengths involved are not the same

* ≠ substance (same conditions) → ≠ spectra

* = substance (different conditions) → = or ≠ spectra

* ALL substances are able of absorbing any electromagnetic radiation

* BUT A little amount of them emitt.

* The wavelengths of light absorbed or emitted by different substance are different

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9. BIBLIOGRAPHY

Principios de Análisis Instrumental, Douglas A. Skoog, Stanley R. Crouch, F. James Holler , Méjico, 2008.