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CERTIFICATION COURSE

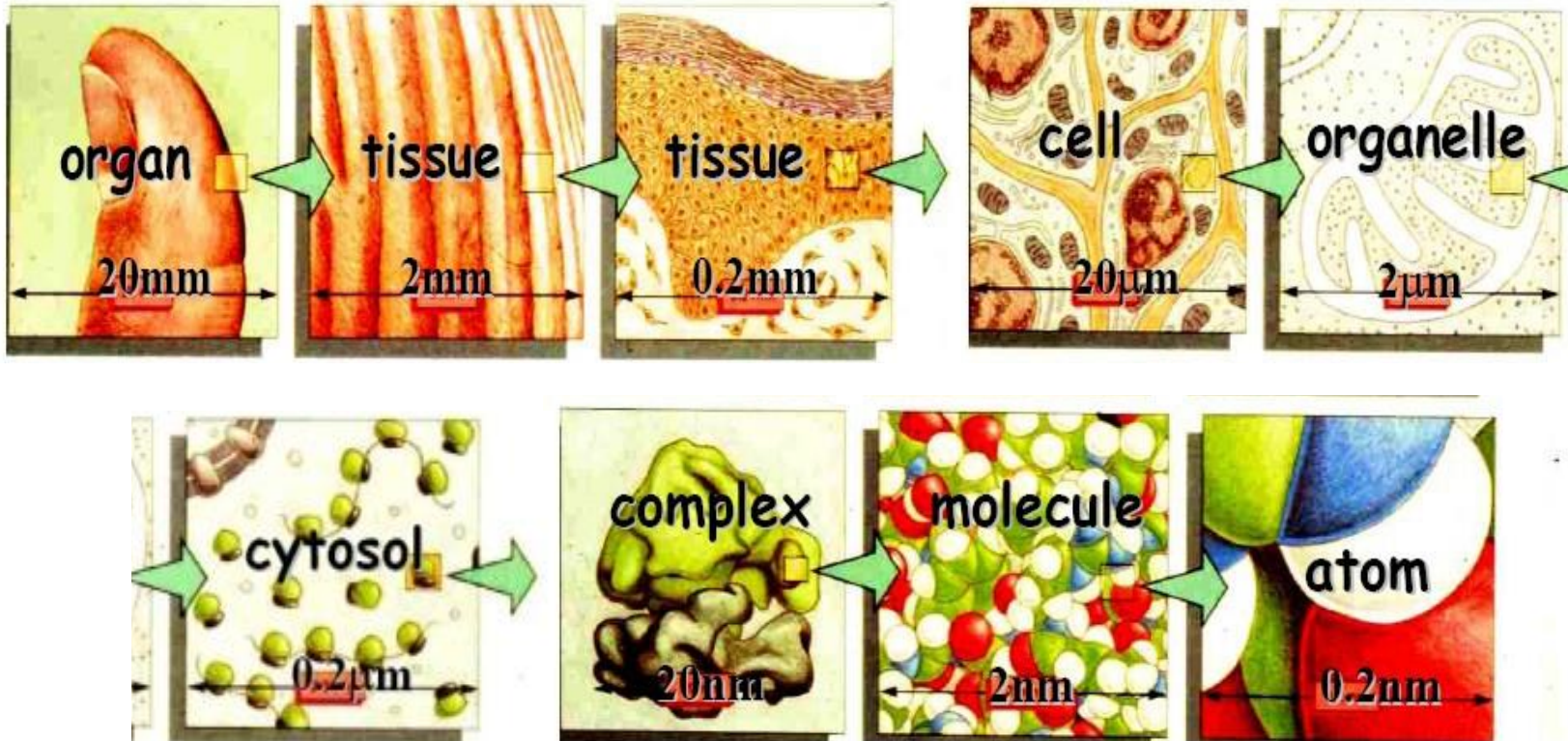
Lecture 19: Review of Biomaterial Optics

Optical Absorption: Cross-section, Hemoglobin & Jaundice detection

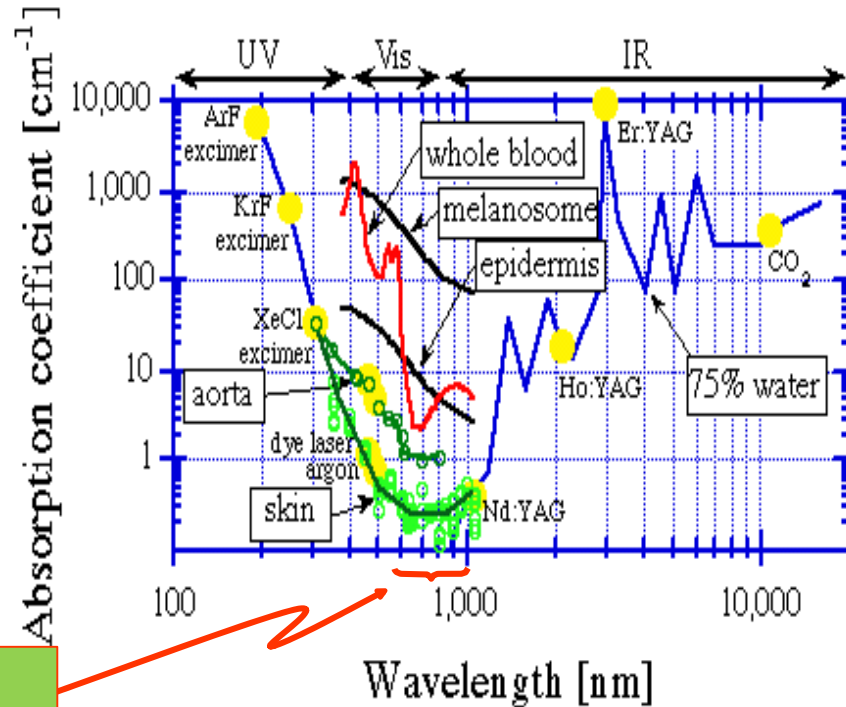
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The Living World



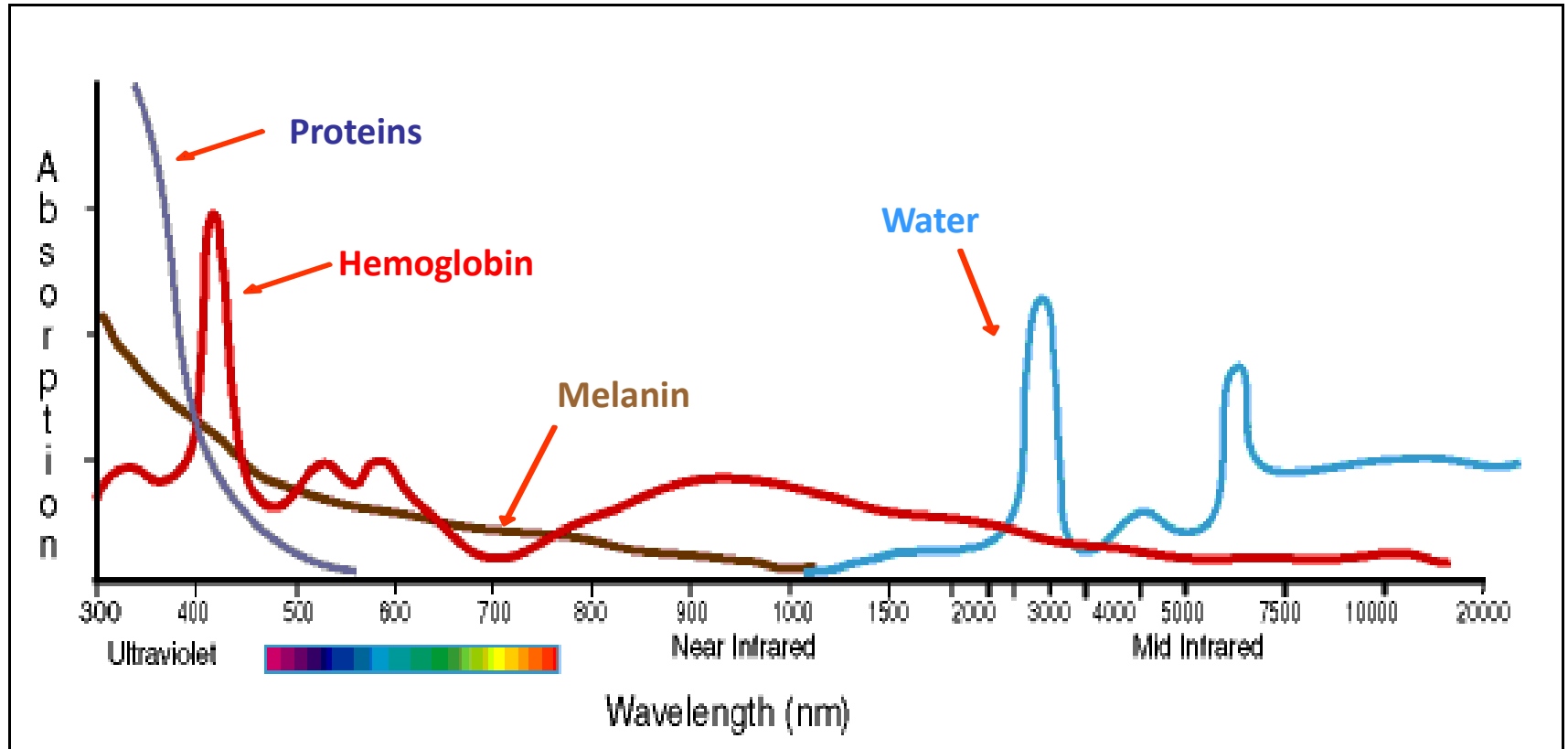
Response of Biomaterials to Optical Radiation - Absorption



Diagnostic and
Therapeutic Window

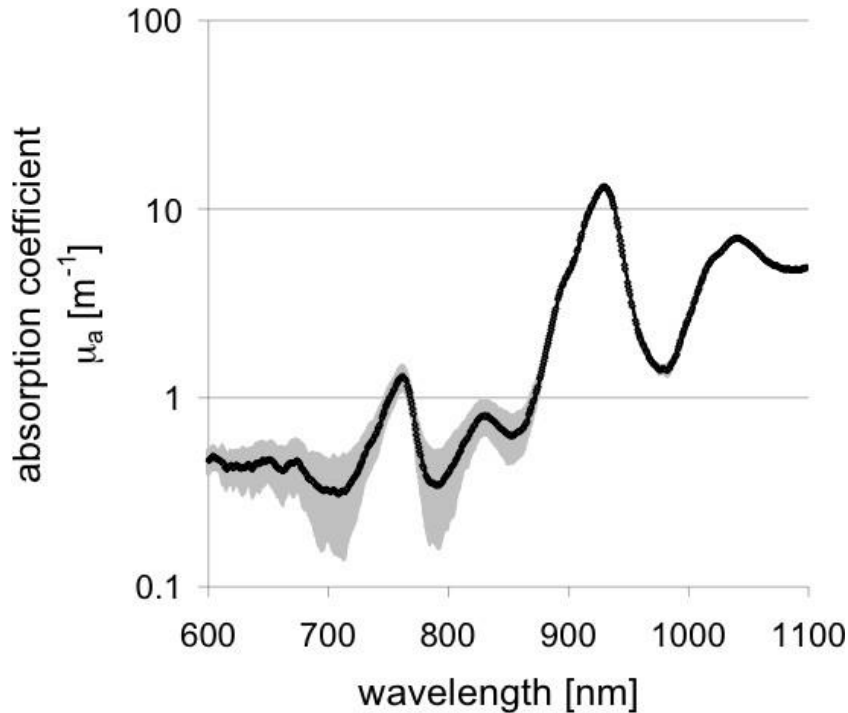
Absorption Curve for Typical Biological Tissues

Tissue Main Absorbers



Response of Biomaterials to Optical Radiation:

Absorption of Fat



Absorption coefficient of fat corrected for scattering contribution versus wavelength. The error bars represent the standard deviation over the 2 temperatures i.e. 37, 60°C

Excitation Process vs. Frequency

THz Range: 0.1- 5THz



Region	Microwave	Far Infrared	Infrared	VIS and UV
Frequency	1 – 100 GHz	0.1 – 30 THz	30 – 435 THz	435 THz – 10 PHz
Wavelength	300 – 3 mm	3 mm – 10 μm	10 μm – 690 nm	690 nm – 30 nm
Wavenumber	0.033 - 3.3 cm^{-1}	3.3 – 1000 cm^{-1}	1000 – 14500 cm^{-1}	14500-333564 cm^{-1}
Energy	4.09×10^{-3} - 0.409 meV	0.409 – 124 meV	124 meV- 1.8 eV	1.8 eV – 41.3 eV
Molecular process	Rotation of Polyatomic molecules	Rotation of small molecules	Vibrations of flexible bonds	Electronic transitions



Definition and Units of Absorption Coefficient μ_a [cm^{-1}]

- Consider a chromophore idealized as a sphere with a particular geometrical size.
- Consider that this sphere blocks incident light and casts a shadow, which constitutes absorption.
- This description is of course an incorrect and schematicized version of the real situation. However, it does provide a simple concept which captures the essence of the absorption coefficient, the parameter we use to describe the effectiveness of absorption.
- The size of the absorption shadow is called the effective cross- section (μ_a [cm^2]) and can be smaller or equal to the geometrical size of the chromophore (A [cm^2]), related by the proportionality constant called the absorption efficiency Q_a [dimensionless]:

$$\mu_a = Q_a A$$

$$[\text{cm}^2] \quad [-][\text{cm}^2]$$

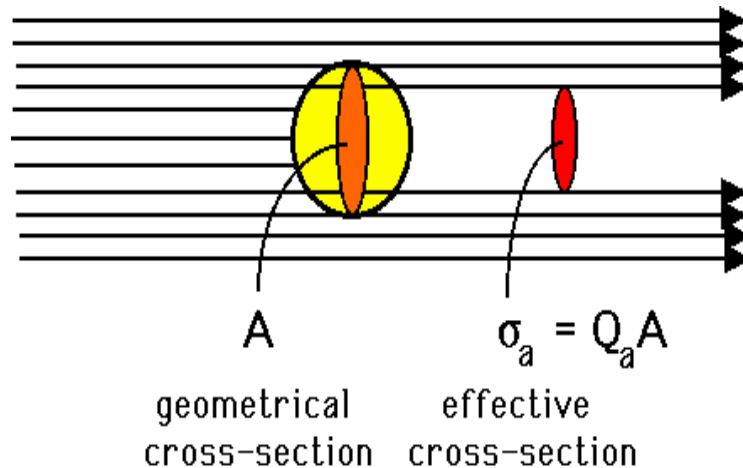
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The **absorption coefficient** μ_a [cm^{-1}] describes a medium containing many chromophores at a concentration described as a volume density μ_a [cm^{-3}]. The absorption coefficient is essentially the cross-sectional area per unit volume of medium.

$$\mu_a = \rho_a \sigma_a$$

[cm^{-1}] [cm^{-3}] [cm^2]



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Experimentally, the units $[\text{cm}^{-1}]$ for μ_a are inverse length, such that the product $\mu_a L$ is dimensionless, where L [cm] is a photon's pathlength of travel through the medium. The probability of survival (or transmission T) of the photon after a pathlength L is:

$$T = \exp[-\mu_a L]$$

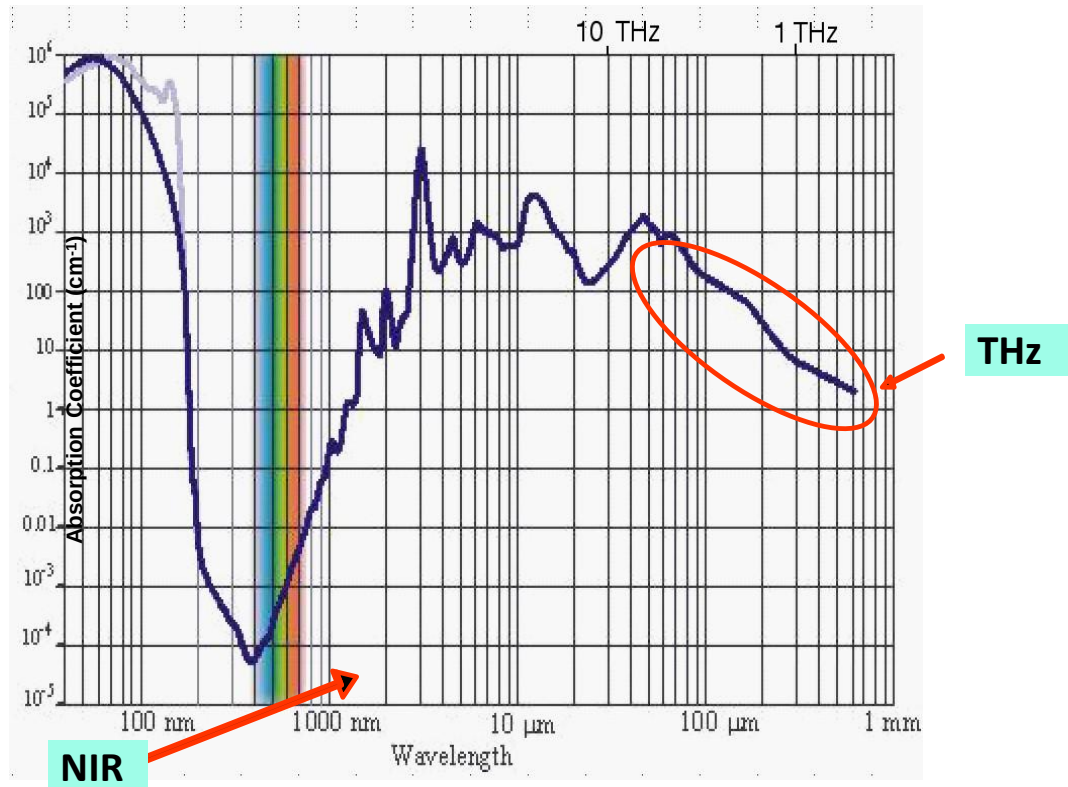
This expression for survival holds true regardless of whether the photon path is a straight line or a highly tortuous path due to multiple scattering in an optically turbid medium.

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Bio-Absorption windows for sensing

- In the ultraviolet, the absorption increases with shorter wavelength due to **protein**, DNA and other molecules.
- In the infrared, the absorption increases with longer wavelengths due to tissue **water** content. Scaling the pure water absorption by 75% mimics a typical tissue with 75% water content.
- In the red to near-infrared (NIR), absorption is minimal. This region is called the **diagnostic and therapeutic window** (originally by John Parrish and Rox Anderson – Wellman labs).

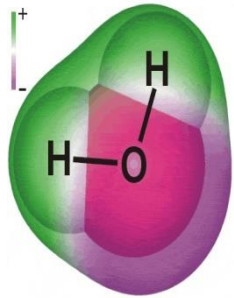
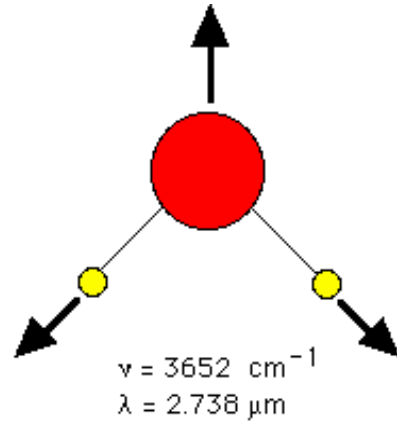
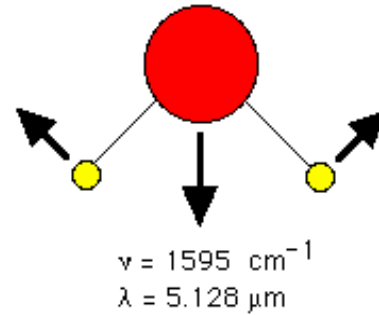
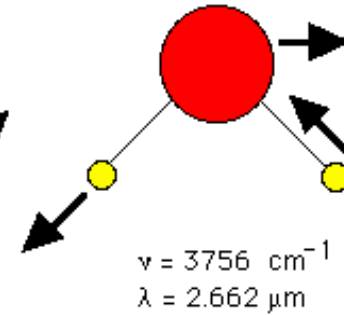
Absorption Spectrum of Water



NIR

THz

Vibrations of Water Molecules



In general the number of vibrational degrees of freedom is $3N-5$ for linear molecules (1D) and $3N-6$ for nonlinear molecules where N is the number of atoms.

Some Important Vibrational Frequencies

Bond	Cycles/cm, ν (1/cm)	Wavelength, $\lambda=1/\nu$ (μm)
C-H stretch	2850-2960	3.378-3.509
C-H bend	1340-1465	6.826-7.462
C-C stretch bend	700-1250	8-14.29
C=C stretch	1620-1680	5.952-6.173
CO_3^{-2}	1410-1450	6.897-7.092
NO_3^-	1350-1420	7.042-7.407
NO_2^-	1230-1250	8.00-8.130
SO_4^{-2}	1080-1130	8.850-9.259
O-H stretch	3590-3650	2.74-2.786
C=O stretch	1640-1780	5.618-6.098
N-H	3200-3500	2.857-3.125



Selected Lasers and Bond Dissociation Energies

Table 3.9. Wavelengths and photon energies of selected laser systems

Laser type	Wavelength (nm)	Photon energy (eV)
ArF	193	6.4
KrF	248	5.0
Nd:YLF (4ω)	263	4.7
XeCl	308	4.0
XeF	351	3.5
Argon ion	514	2.4
Nd:YLF (2ω)	526.5	2.4
He-Ne	633	2.0
Diode	800	1.6
Nd:YLF	1053	1.2
Nd:YAG	1064	1.2
Ho:YAG	2120	0.6
Er:YAG	2940	0.4
CO ₂	10600	0.1

Table 3.8. Dissociation energies of selected chemical bonds. Data according to Pauling (1962)

Type of bond	Dissociation energy (eV)
C=O	7.1
C=C	6.4
O-H	4.8
N-H	4.1
C-O	3.6
C-C	3.6
S-H	3.5
C-N	3.0
C-S	2.7

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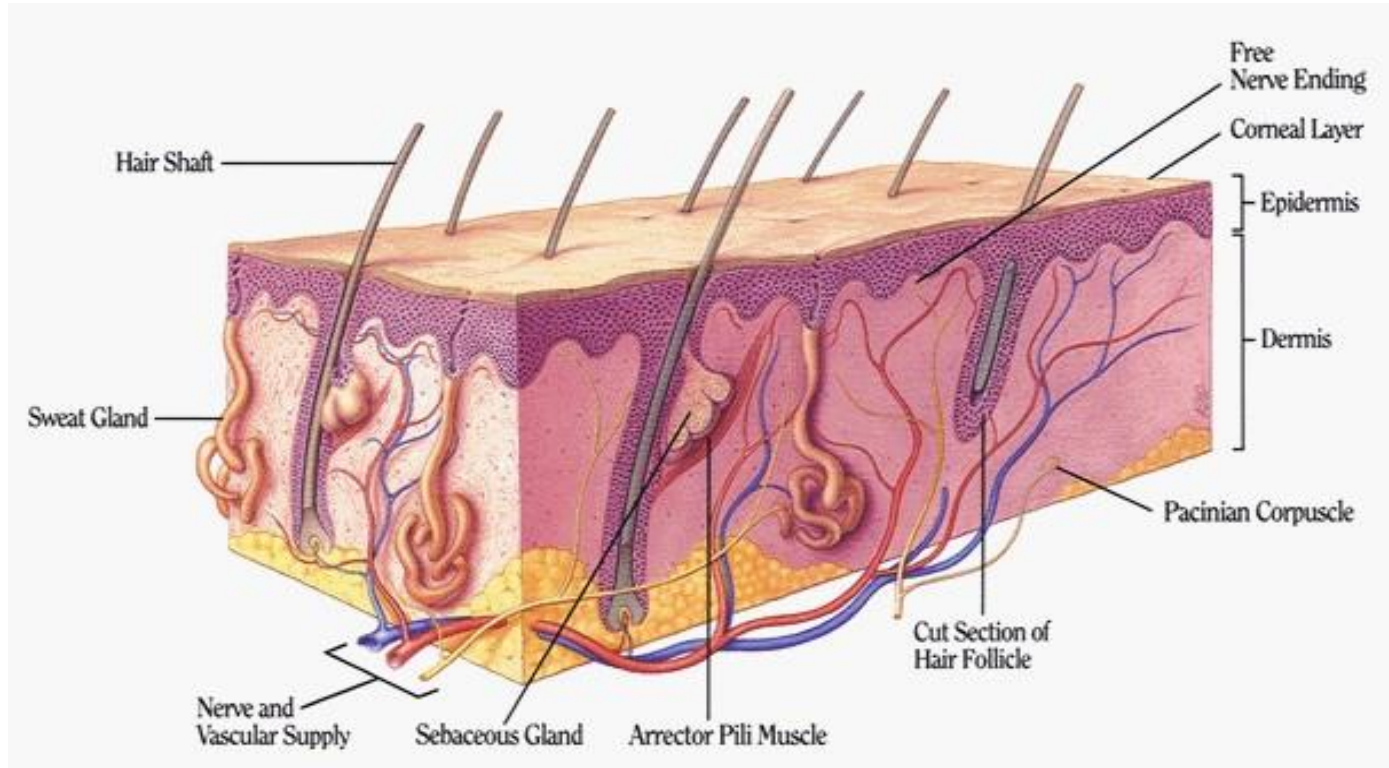
Absorption – Cont'

- Whole blood is a strong absorber in the red-NIR regime, but because the volume fraction of blood is a few percent in tissues, the average absorption coefficient that affects light transport is moderate. However, when photons strike a blood vessel they encounter the full strong absorption of whole blood. Hence, local absorption properties govern light- tissue interactions, and average absorption properties govern light transport.

Melanosomes are also strong absorbers. However, their volume fraction in the epidermis may be quite low, perhaps several percent. So again, the local interaction of light with the melanosomes is strong, but the melanosome contribution to the average absorption coefficient may modestly affect light transport

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Skin Layered Structure

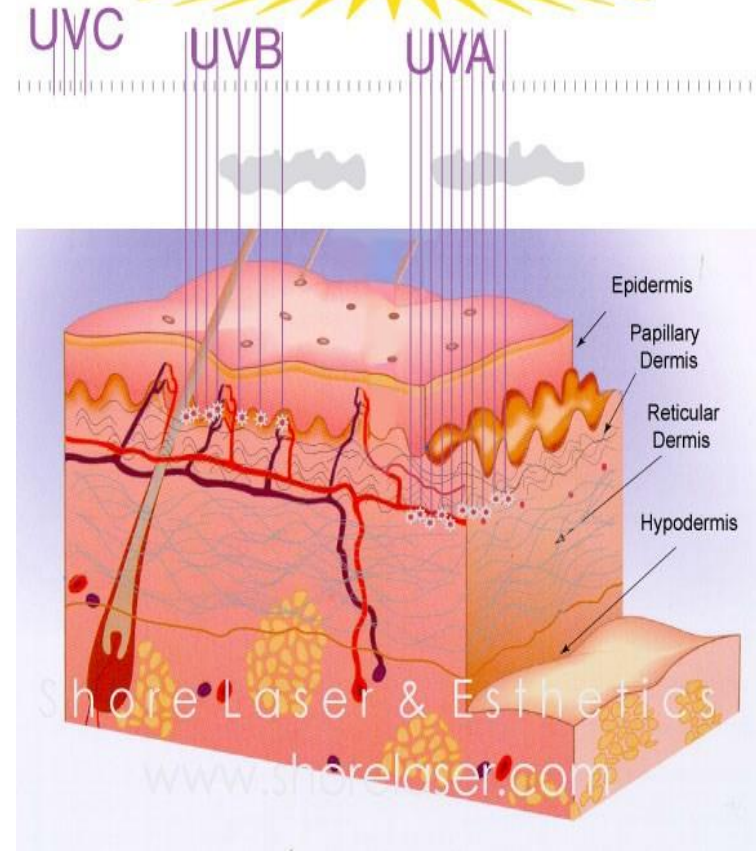


UV Effects on Skin

UVC (200-290nm)- Blocked by the Ozone layer

UVB (290-320nm)- The worse in the summer and in midday. The shorter wave UVB damages the upper layers (epidermis) of skin, and is the primary cause of tanning, sunburn, and skin cancer. UVB is partially blocked by clouds and the atmosphere, which is why one is less likely to burn in cloudy days, in the winter, or in more northern climates.

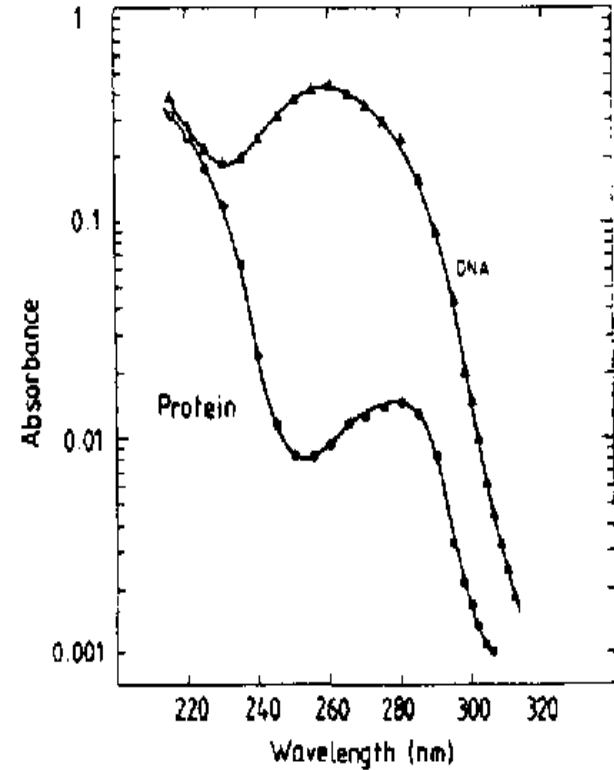
UVA (320-400nm) - Long wave ultraviolet rays which penetrate deeply into the skin to damage collagen and elastic fibers. UVA rays penetrate through clouds and atmosphere (window glass, too!) and deeply into the skin, to damage connective tissue elements and blood vessels in the delicate upper dermis, even in the morning and evening, while driving, and in the winter when the sun is lower in the sky. *One can think of UVB as causing skin cancer, and UVA as the primary cause of photoaging.*



UV Effects on Skin II : Nucleic Acids Absorption

It is the nucleotide bases that are the chromophores (absorbing centres) within nucleic acids. In deoxyribonucleic acid (DNA) these bases are the purine derivatives adenine and guanine, and the pyrimidine derivatives thymine and cytosine. Although the absorption spectra of the component bases differ slightly, their common features are an absorption maximum between 260-265 nm with a rapid reduction in absorption at longer wavelengths

Proteins have similar absorption at 280nm

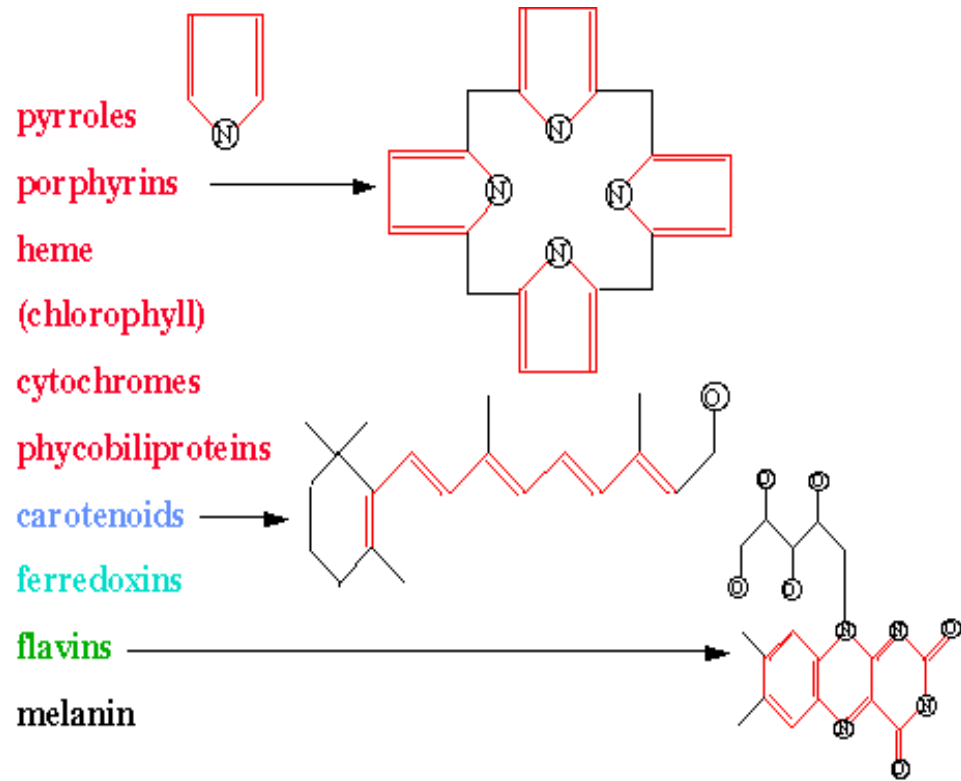


Diffey, B. L. Review in *Physics in Medicine and Biology* 36 (3): 299 (1991)



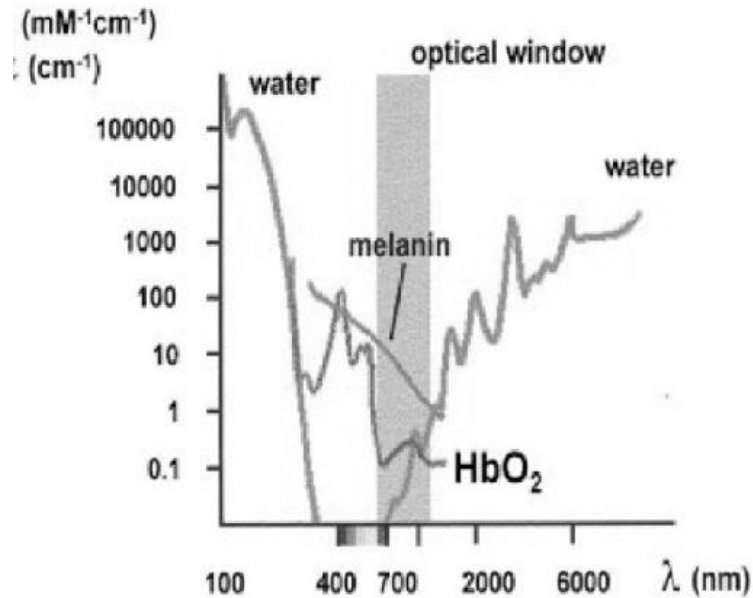
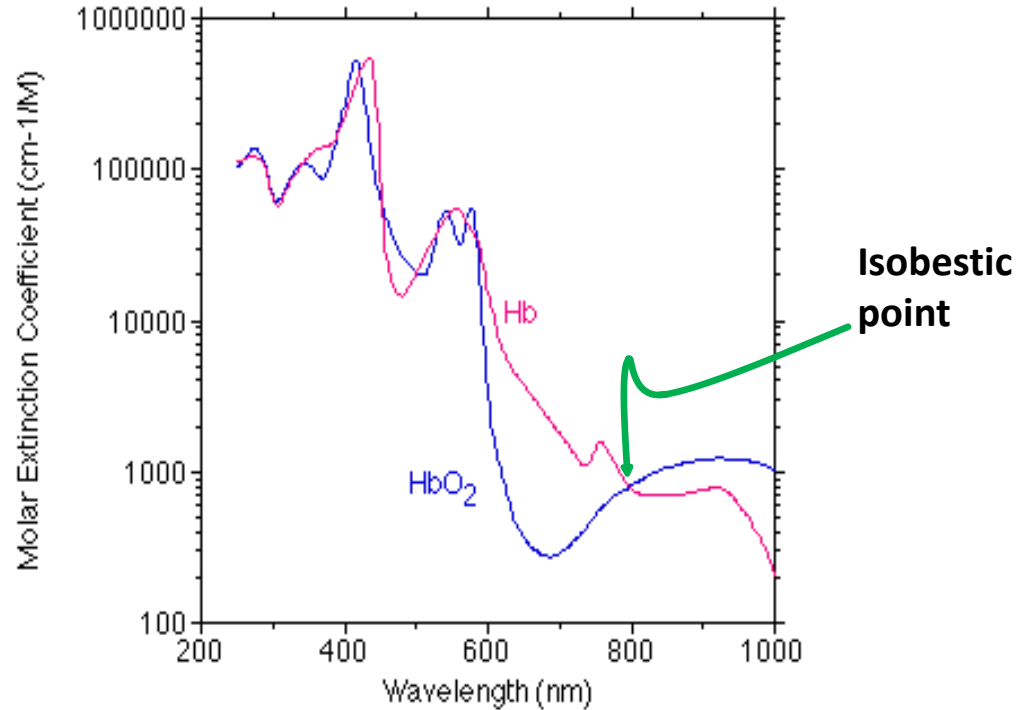
Biological Chromophores

- In early biological evolution, the pyrrole molecule was a chromophore which could absorb sunlight which enabled subsequent synthetic reactions that produced biological polymers and other proto-metabolic products.
- Combining four pyrroles into a tetrapyrrole ring (porphyrin) yielded an efficient chromophore for collecting solar photons. Chlorophyll is such a porphyrin. Hemoglobin, vitamin B12, cytochrome C, and P450 are also examples of porphyrins in biology.



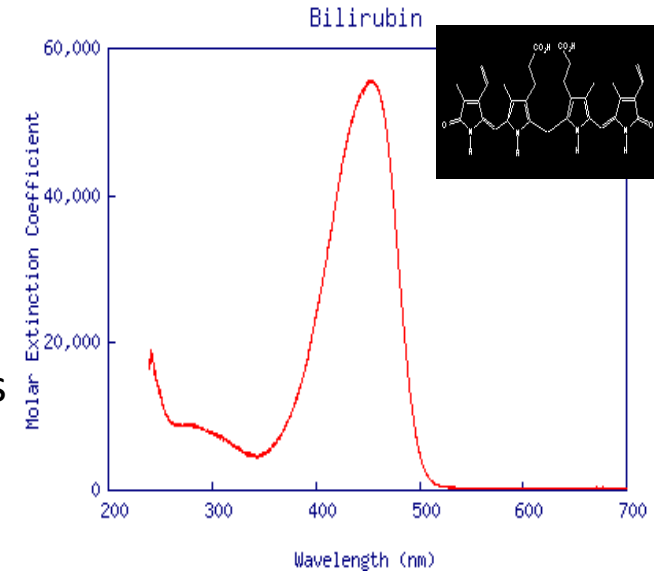
Absorption Spectra of Hb and HbO₂

Very Important for Oxymetry !



Another Important Example: Bilirubin

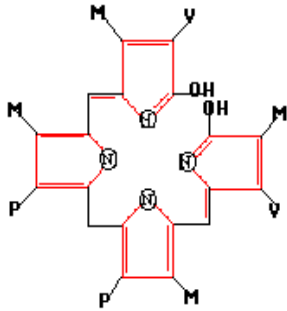
- A chromophore encountered when a newborn infant suffers from "jaundice", a syndrome in which the skin presents a yellow color.
- A breakdown product of hemoglobin. Often there is significant hemolysis of red blood cells during child birth contributing to a transient bilirubin load.
- Normally, bilirubin binds to the serum protein albumin and is carried to the liver where enzymes convert it into a water-soluble form which is removed from the blood into the bile. But in newborns who have not yet developed sufficient enzymes to accomplish this task, the bilirubin accumulates in the blood, exceeds the holding capacity of the albumin, and spills into the skin to give the yellow skin color, and into the brain to cause irreversible brain damage (kernicterus).



A typical jaundiced neonate has a bilirubin concentration of 10 mg/dL and the molecular weight for bilirubin is 574.65g/mole.



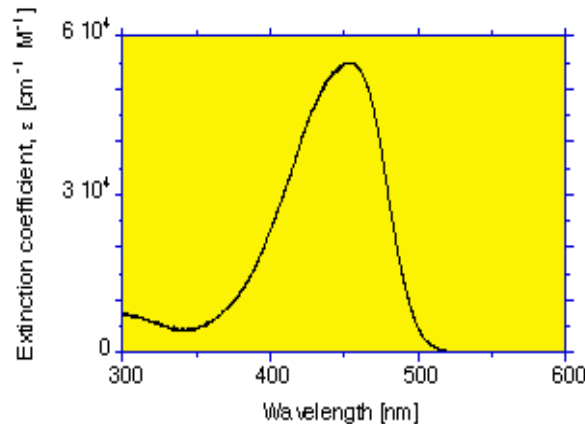
Approx. Estimation of: A , ρ_a , μ_a , Q_a , and σ_a for Bilirubin



The structure of bilirubin is shown.

The diameter is approximately 1 nm.

So the geometrical area is $A = 4.5 \times 10^{-15} \text{ cm}^2$.



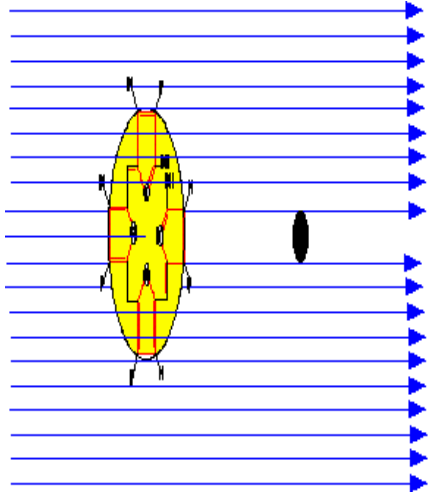
At 460 nm, the extinction coefficient of bilirubin is = 53,846 [$\text{Liter} \cdot \text{cm}^{-1} \text{M}^{-1}$] (see Characteristic curve).

A typical jaundiced neonate might have a bilirubin concentration of 10 mg/dL, or

$$(0.100 \text{ g/liter}) / (574.65 \text{ g/mole}) = 0.17 \times 10^{-3} \text{ M/L}$$

In such a case, the bilirubin absorption coefficient at 460 nm is roughly:

$$\mu_a = \epsilon c \ln(10) = (53846 \text{ [L.cm}^{-1}\text{M}^{-1}])(0.17 \times 10^{-3} \text{ M/L})(2.3) = 21 \text{ cm}^{-1}.$$



The concentration c is equivalent to: $\rho_a = (0.17 \times 10^{-3} \text{ [moles/liter]}) \times (6 \times 10^{23} \text{ [mole}^{-1}\text{]}) / (1000 \text{ cm}^3/\text{liter}) = 1.02 \times 10^{17} \text{ [cm}^{-3}\text{]}$

Efficiency of absorption:

$$Q_a = \mu_a / (\rho_a A) = (21 \text{ [cm}^{-1}\text{]}) / ((1.02 \times 10^{17} \text{ [cm}^{-3}\text{])}(A = 4.5 \times 10^{-15} \text{ [cm}^2\text{]}) = 0.046$$

Effective cross-section: $\sigma_a = Q_a A = (0.046)(4.5 \times 10^{-15} \text{ [cm}^2\text{]}) = 2.1 \times 10^{-16} \text{ [cm}^2\text{]}.$

Bilirubin's effective cross-sectional diameter is $\sqrt{0.046}$ or 21% the size of its geometrical diameter.

Summary

1. Various optical absorption domains for tissues were presented
2. Absorption coefficient was discussed
3. Effect of UV on skin was analyzed
4. Hb detection and jaundice detection were treated analytically using optical absorption cross-section technique.

Thank You