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from this link



quantum mechanics on the supermarket shelf

how theoretical physics helped design a healthier colorant for popular candies

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Trieste — Italy

natural dyes in the food industry

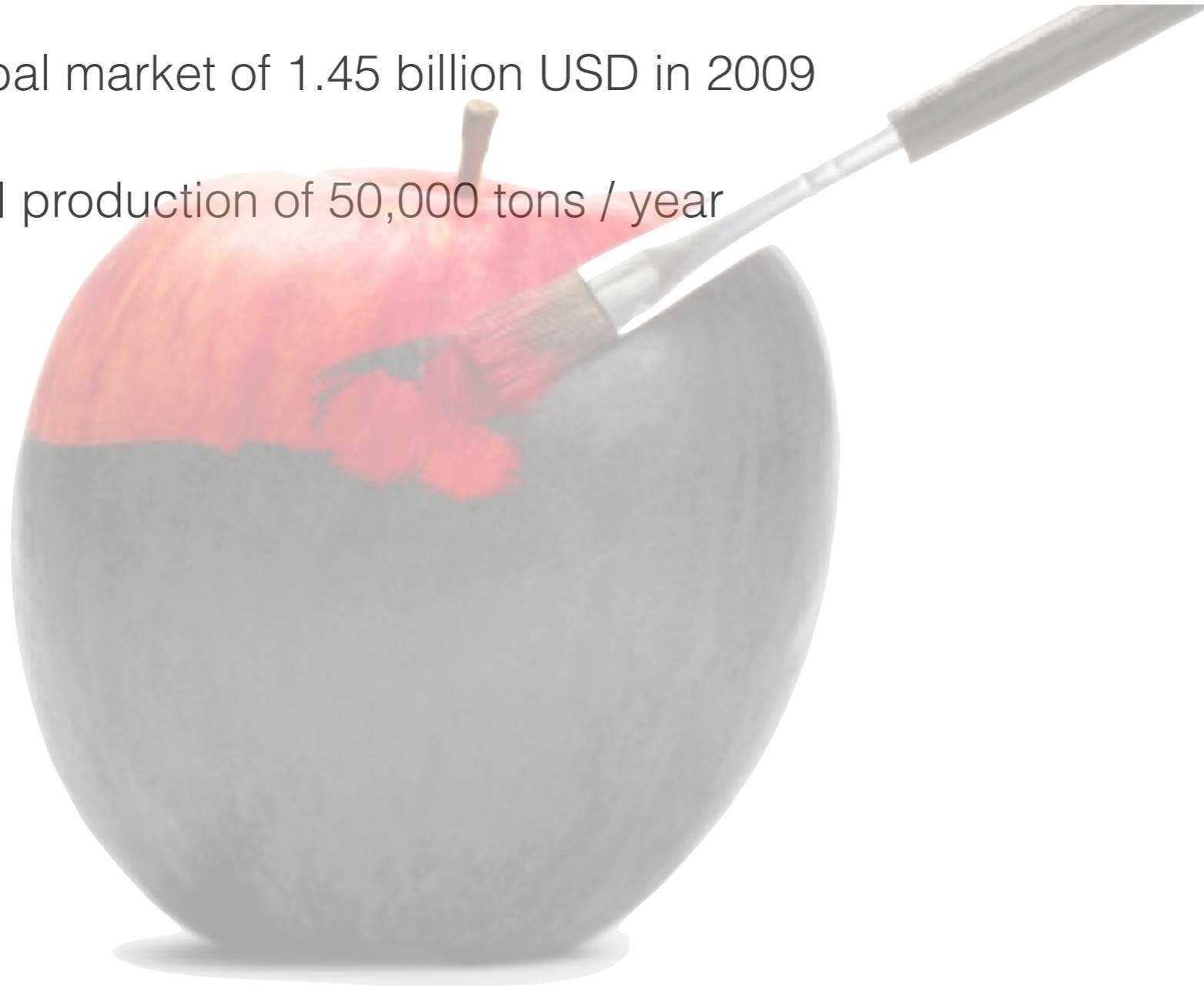


MAX

natural dyes in the food industry

👉 global market of 1.45 billion USD in 2009

👉 total production of 50,000 tons / year



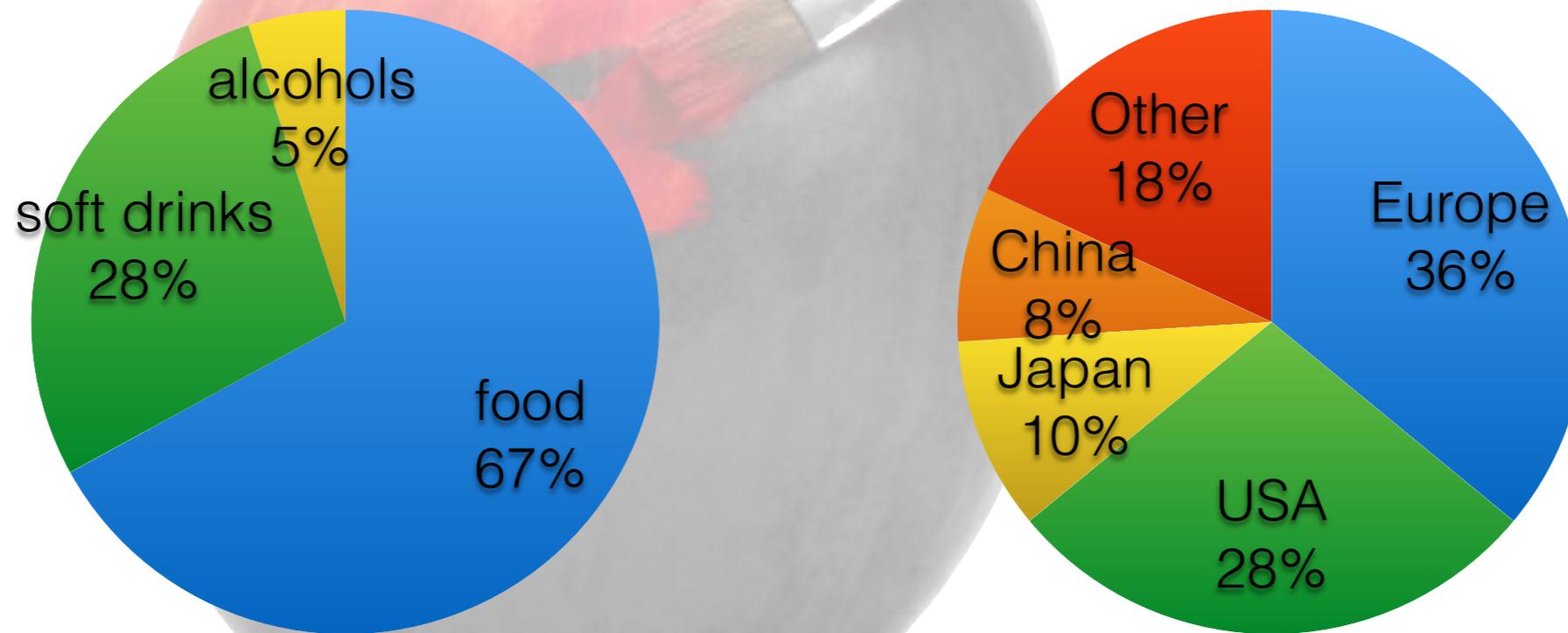
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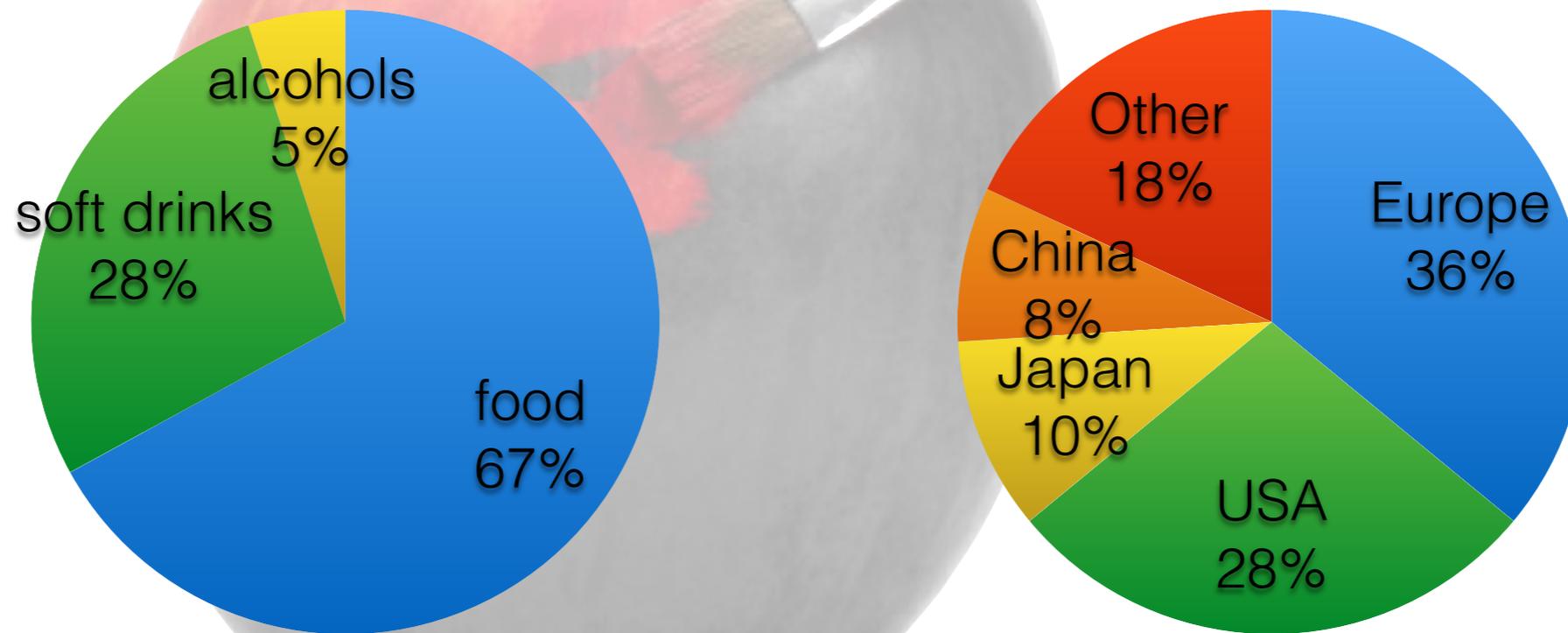
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natural dyes market grown by 35% in the 2005-2009 quinquennium

the food industry is subject to an increasing global pressure from customers and legislators who demand a shift towards ingredients and additives that are perceived as *more natural* and, “therefore”, *healthier*

natural dyes: the requirements

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- tunable

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- stable

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- tunable
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- inexpensive

the Southampton six

In 2007 Research funded by the UK FSA was published, suggesting that the consumption of certain mixes of artificial food colours and preservatives could be linked to attention deficit and increased hyperactivity in some children.



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Box A: The Seven
Southampton Additives

Colours:

-  Tartrazine (E102)
-  Quinoline yellow (E104)
-  Sunset yellow (E110)
-  Carmoisine (E122)
-  Ponceau 4R (E124)
-  Allura red (E129)

Preservative:

-  Sodium benzoate (E211)

Since 2010 an EU-wide compulsory warning must be put on any food and drink product that contains any of these six colours:

“May have an adverse effect on activity and attention in children”

M&M'S

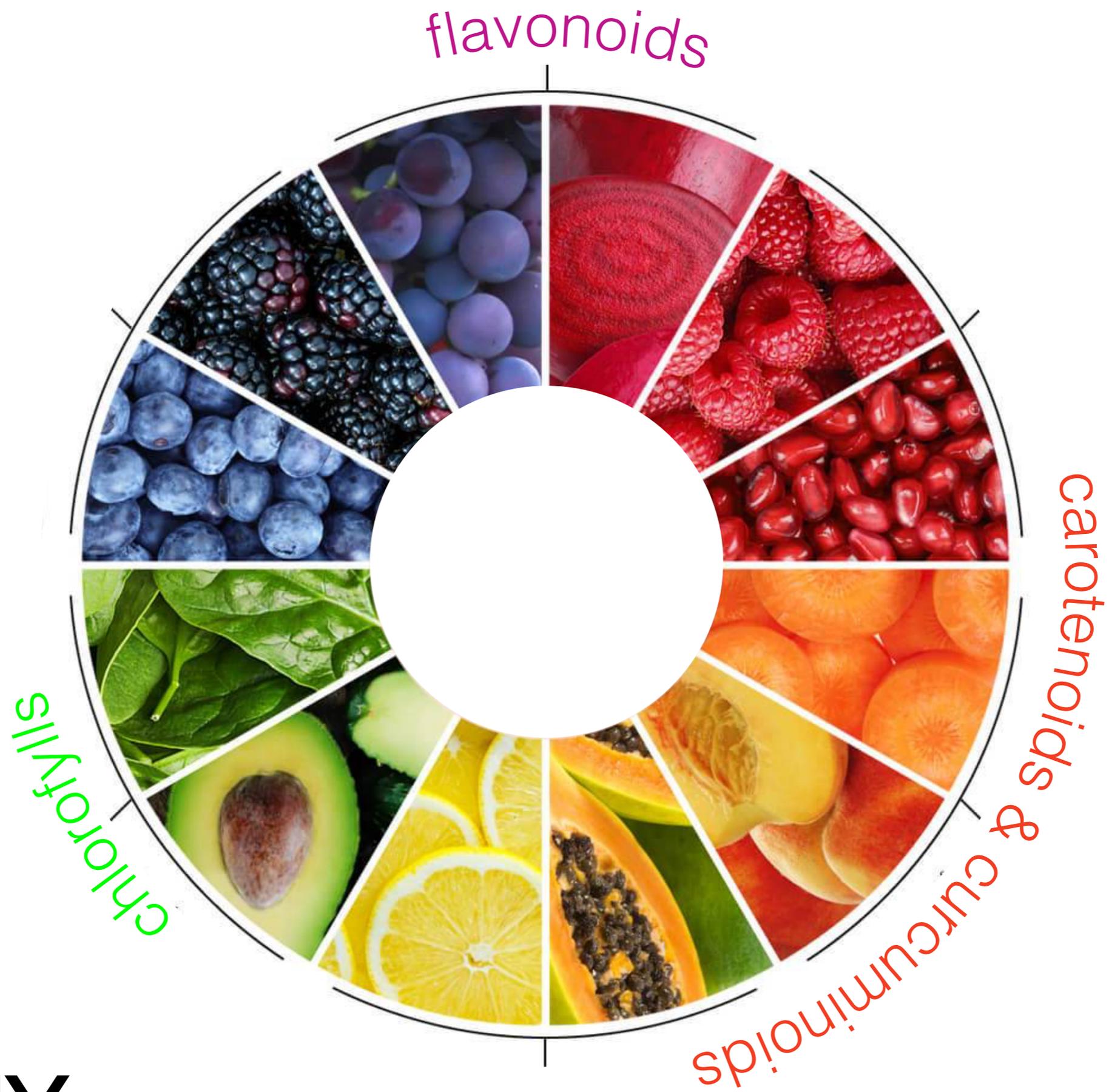
chocolate
north america

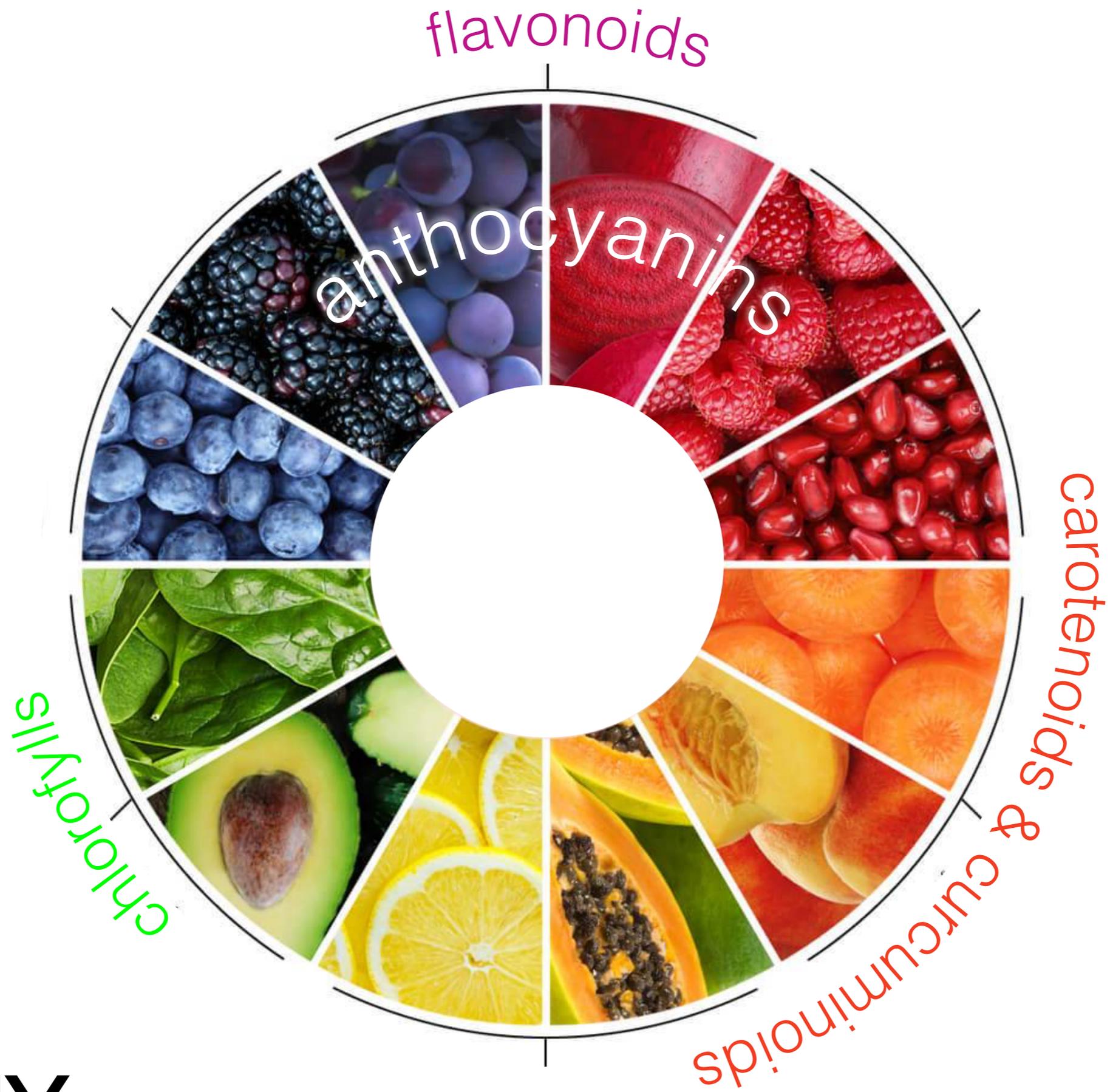


M&M'S

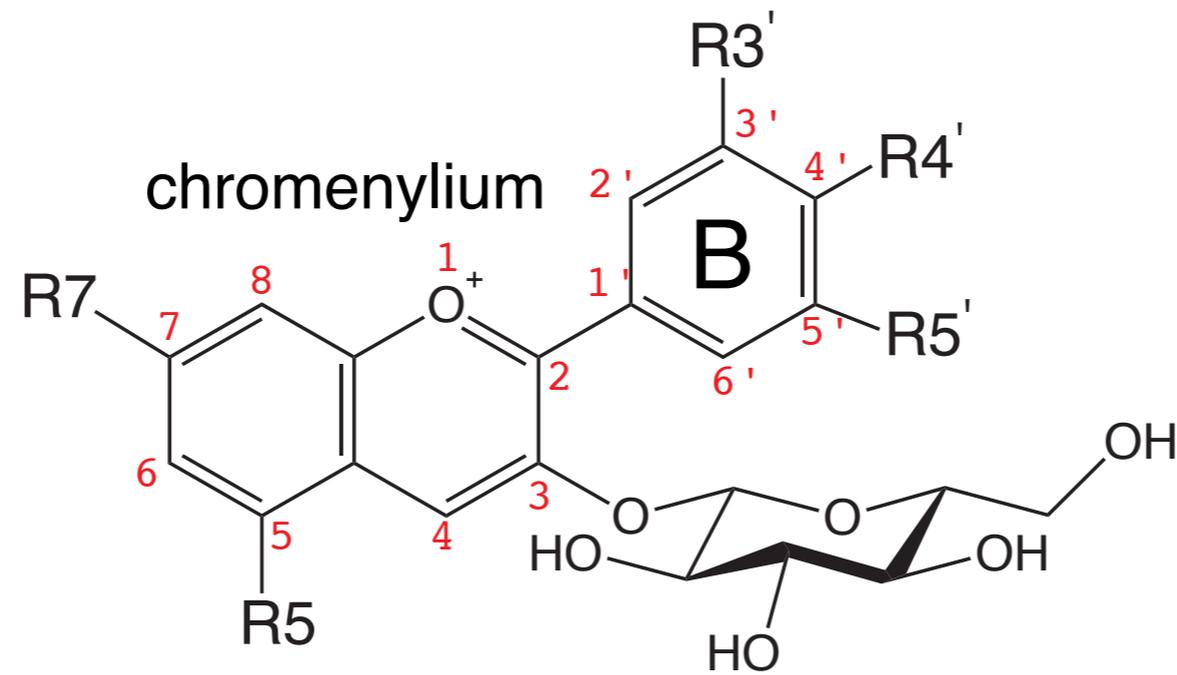
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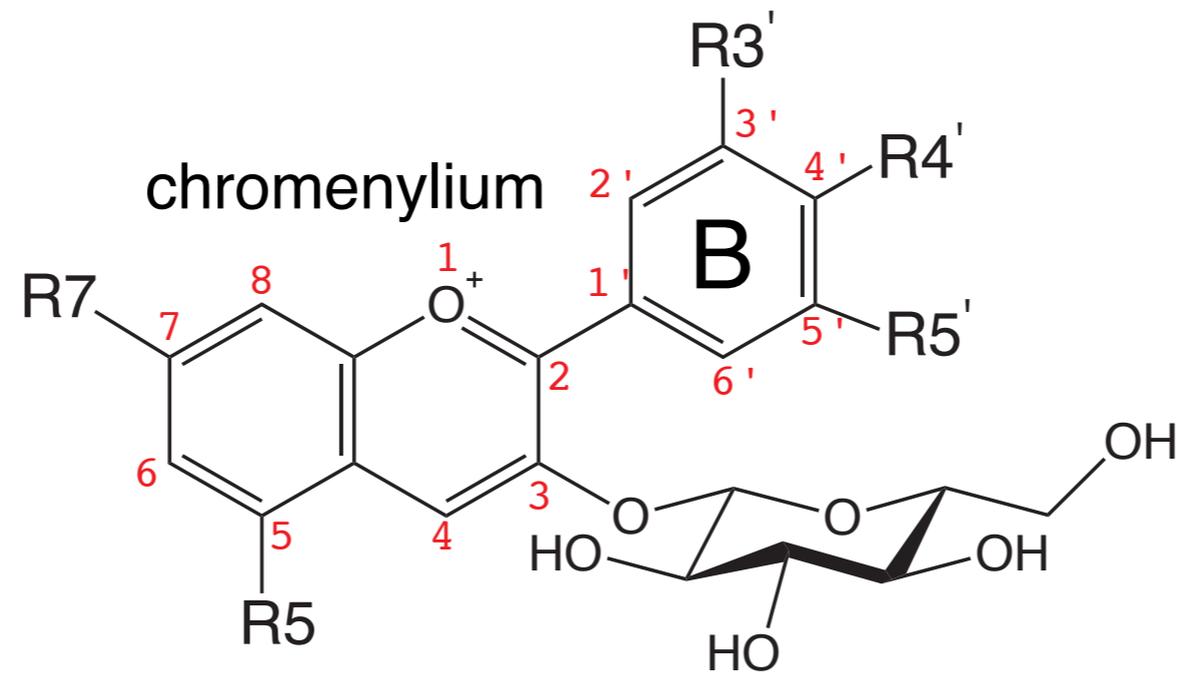
anthocyanins



anthocyanin	R3'	R4'	R5'	R7
cyanin	-OH	-OH	-H	-OH



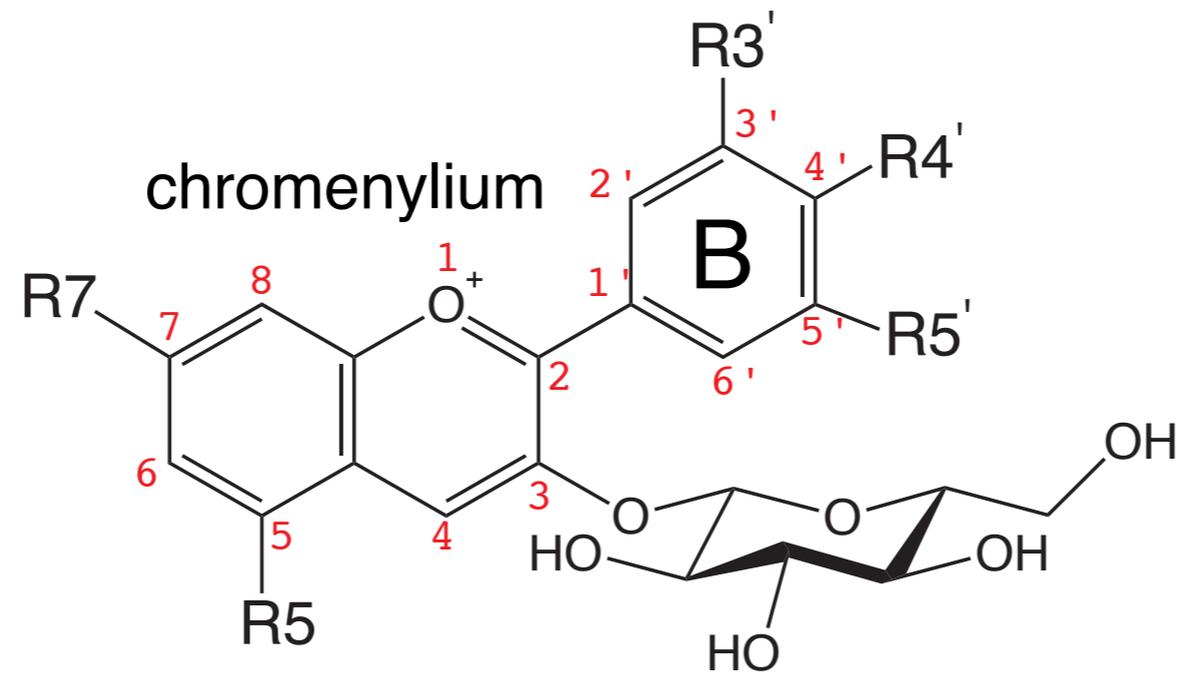
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peonin	-OCH ₃	-OH	-H	-OH



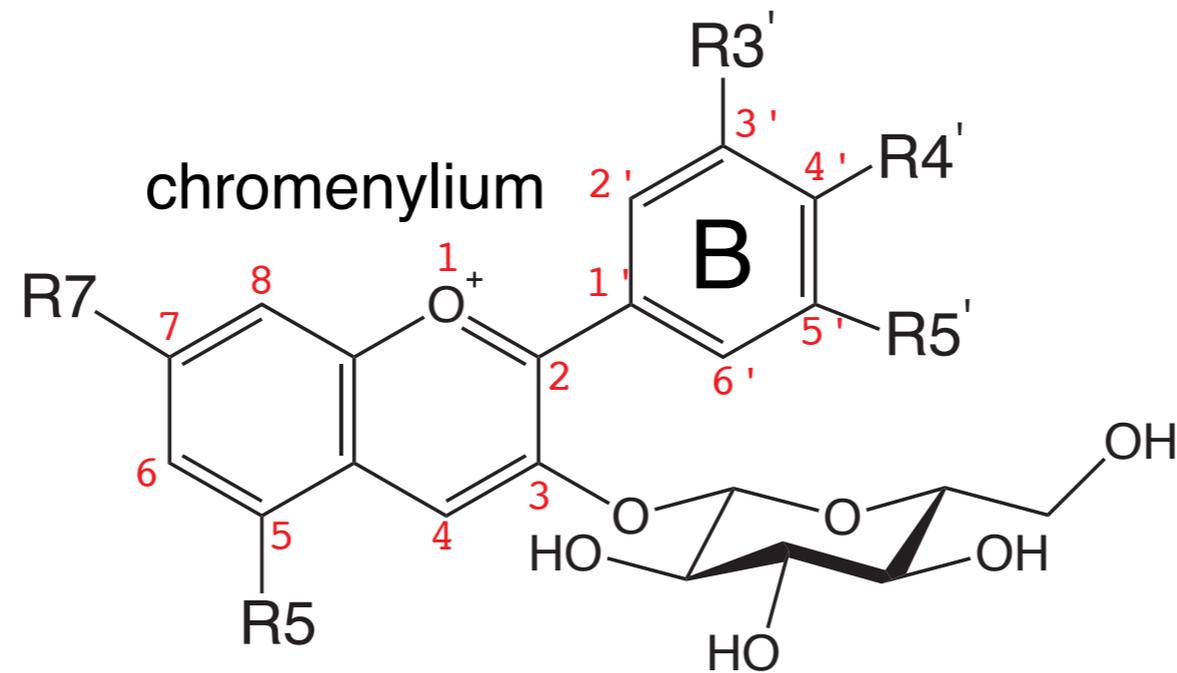
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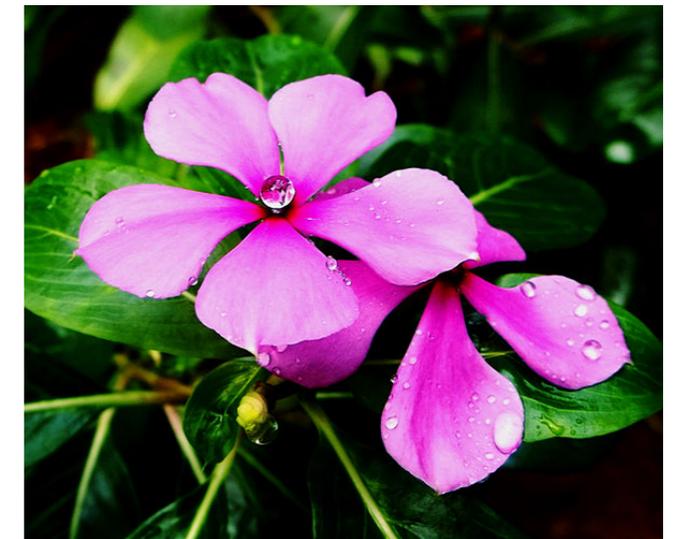
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peonin	-OCH ₃	-OH	-H	-OH
rosinin	-OH	-OH	-H	-OCH ₃



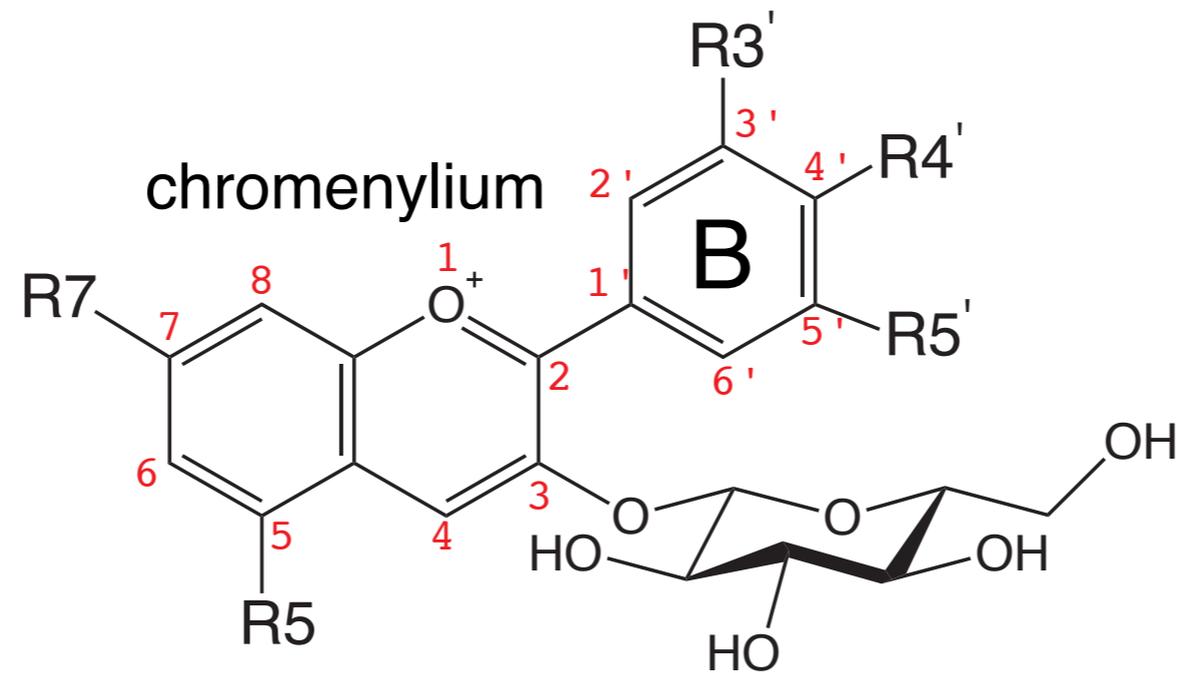
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malvin	-OCH ₃	-OH	-OCH ₃	-OH



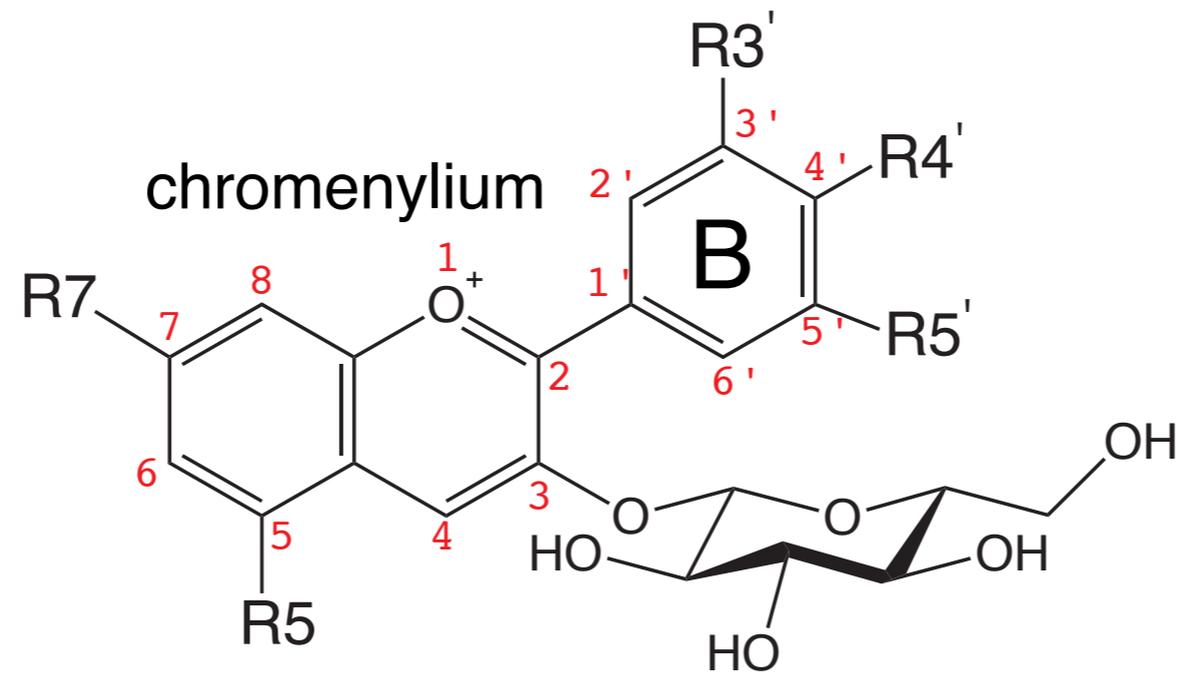
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delphinin	-OH	-OH	-OCH ₃	-OH



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malvin	-OCH ₃	-OH	-OCH ₃	-OH
delphinin	-OH	-OH	-OCH ₃	-OH
pelargonin	-H	-OH	-OH	-OH



anthocyanin: the hurdles towards a rational design

anthocyanin: the hurdles towards a rational design

- the stability and color function of anthocyanins are affected by many and diverse factors:
 - chemical diversity (phenols, sugars, and acylation);
 - acidity of the solution;
 - co-pigmentation;

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- the high reactivity of the phenolic chromophore makes synthesis extremely difficult and the product often unstable:
 - very little research is being done in this area;
 - most of it simply aims at isolating from natural sources (highly expensive and difficult);



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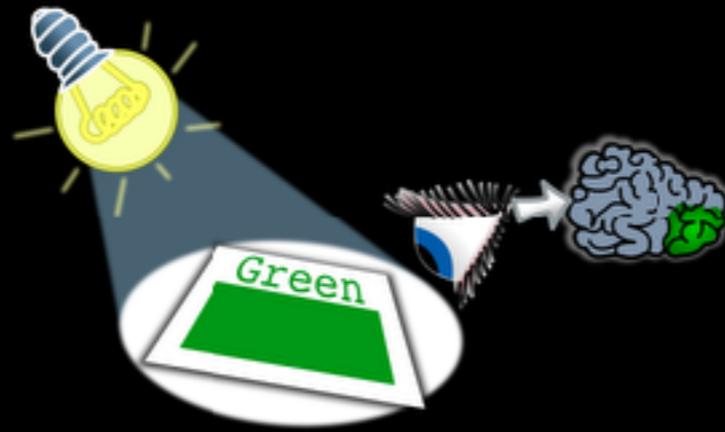
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- very little is known of the microscopic mechanisms that determine the stability and the chromatic properties of anthocyanins and the relation between structure and color.



MAX

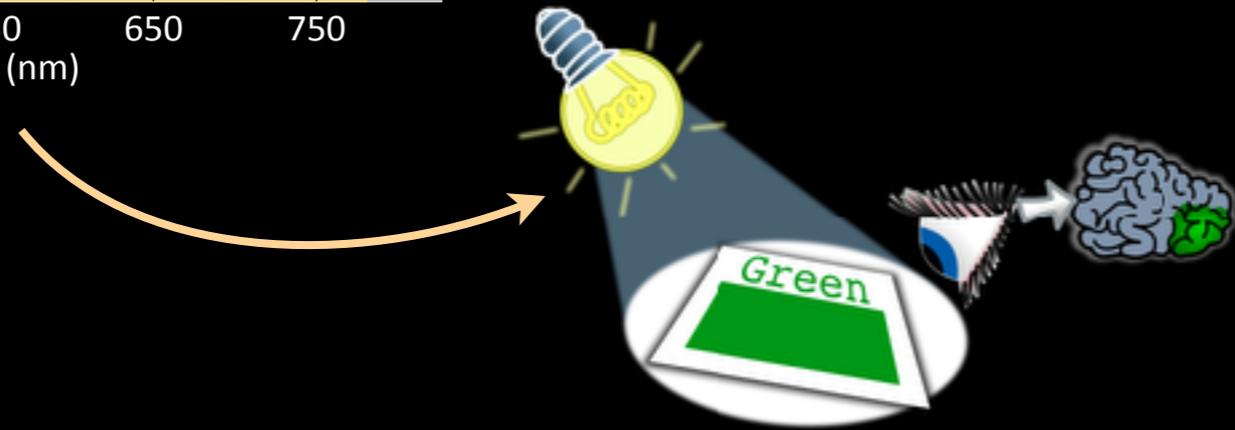
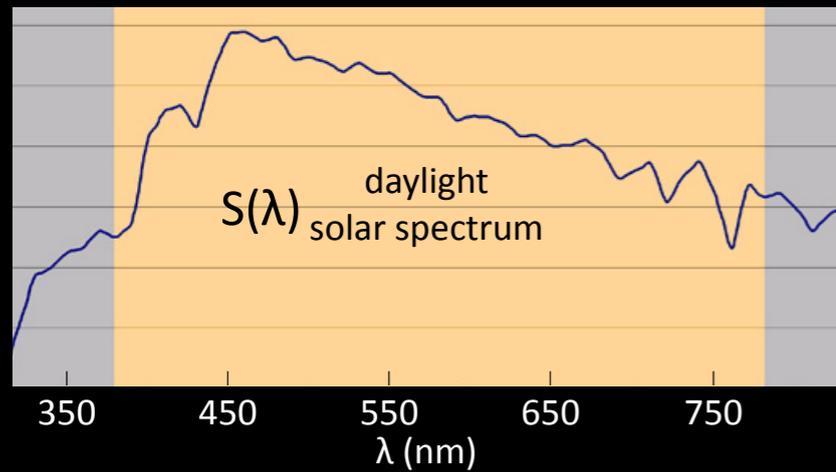
what color is all about



stimulus =

illuminant × transmission × sensitivity

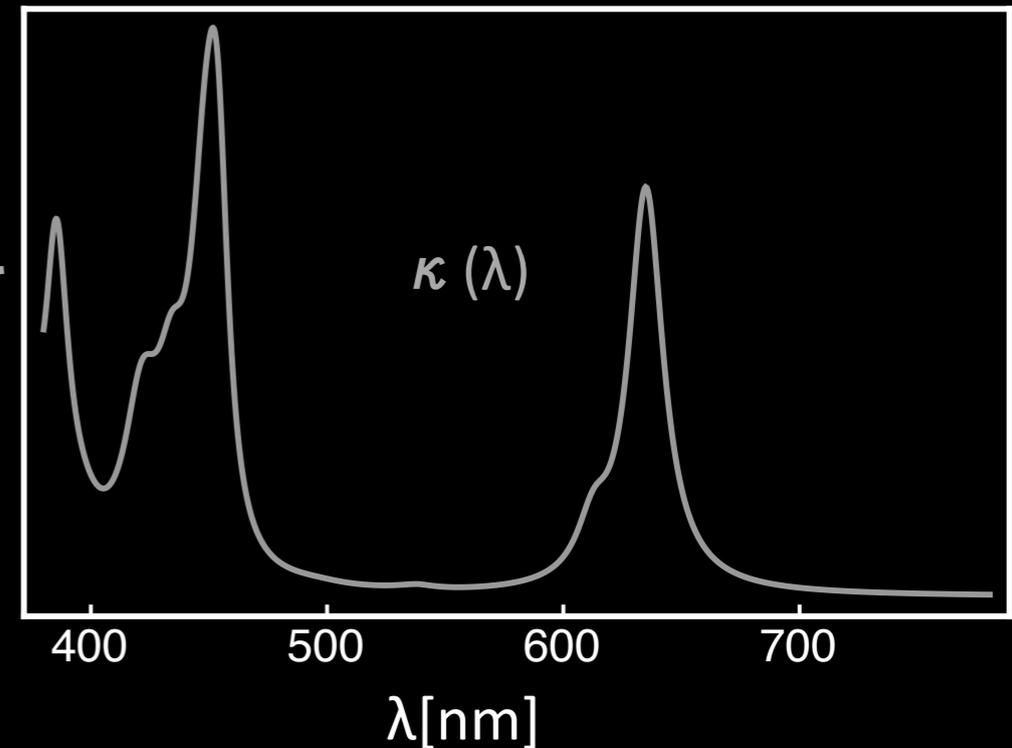
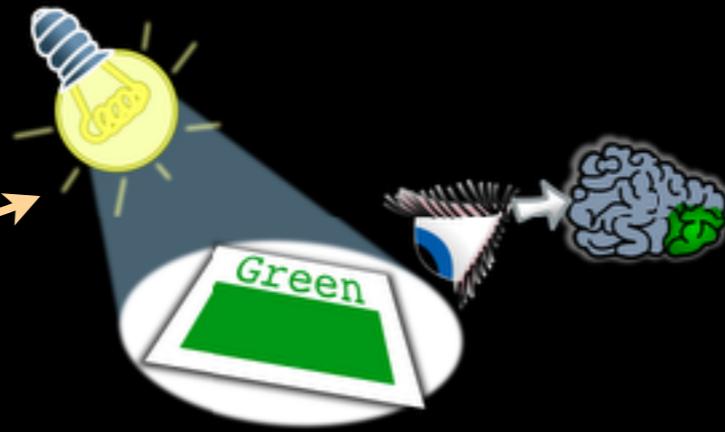
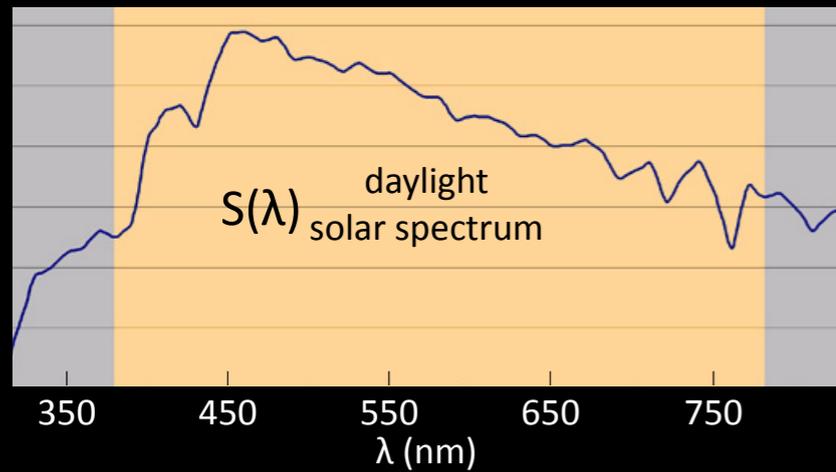
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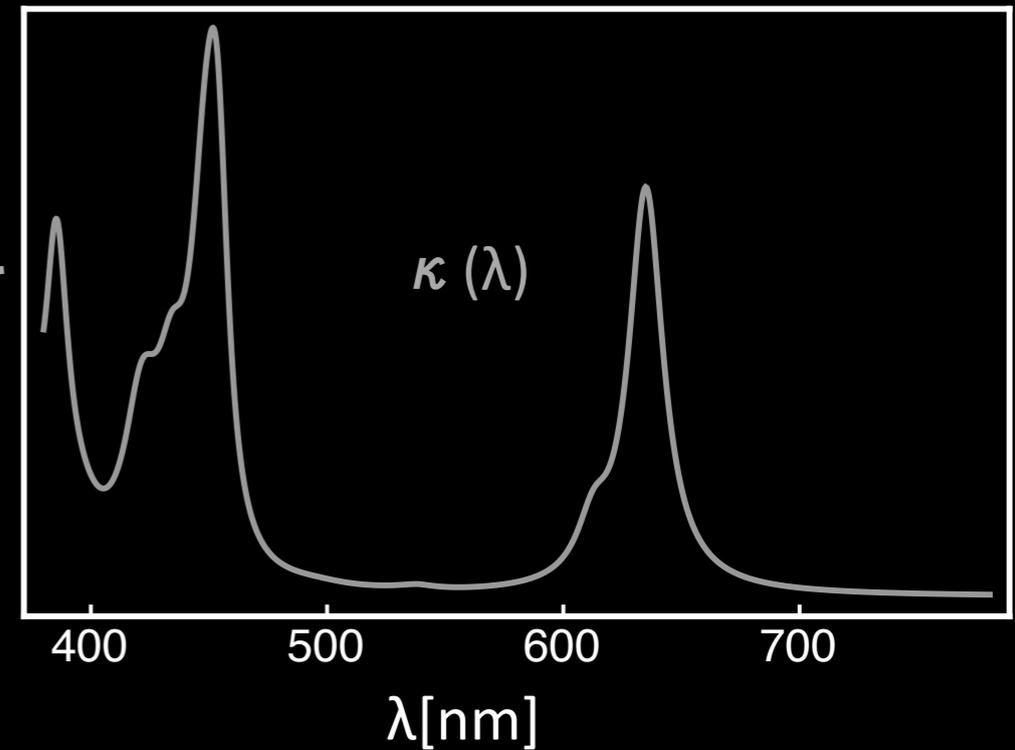
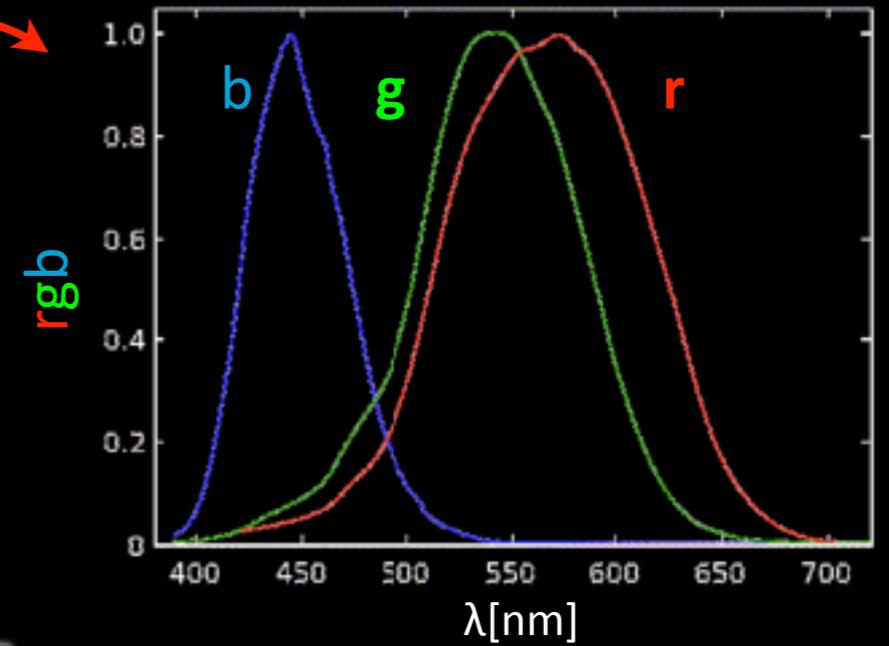
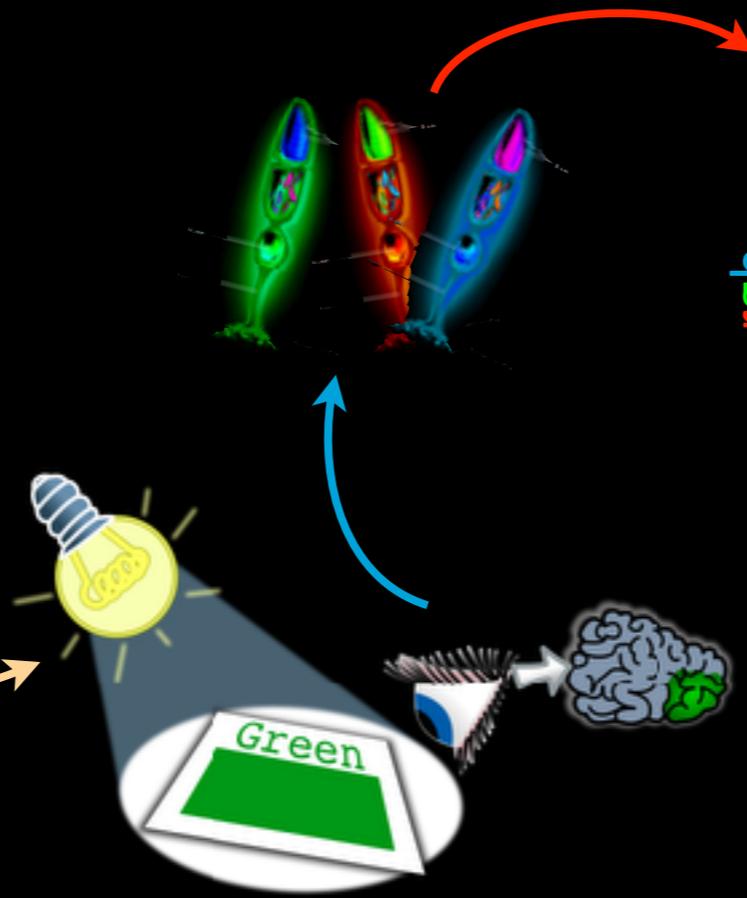
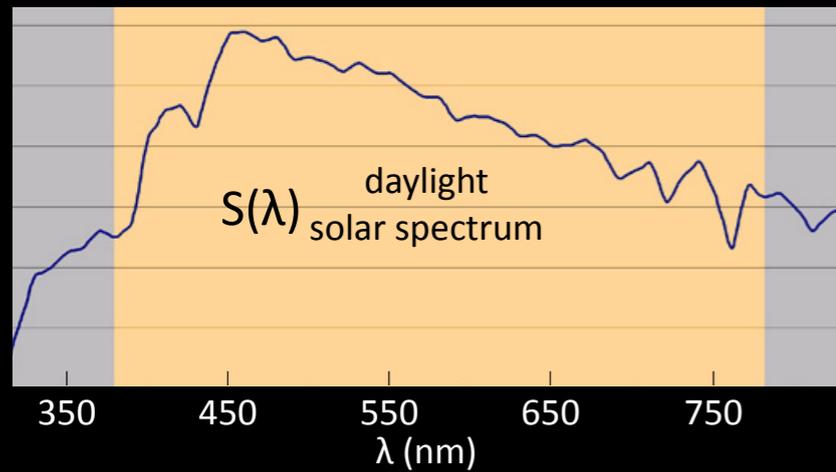
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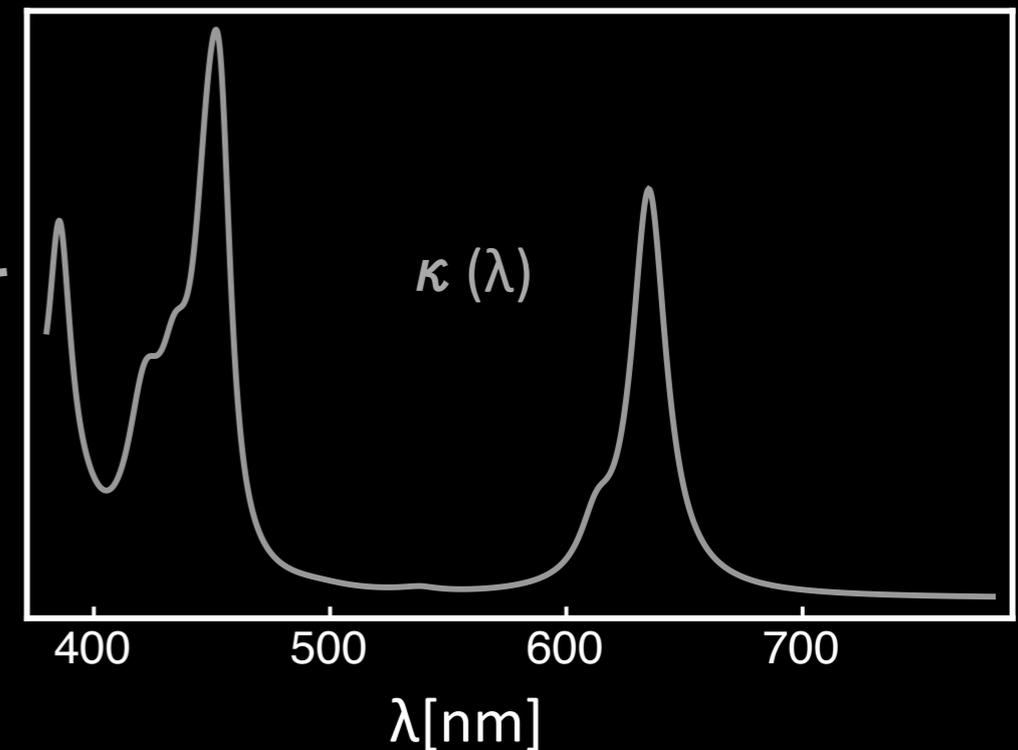
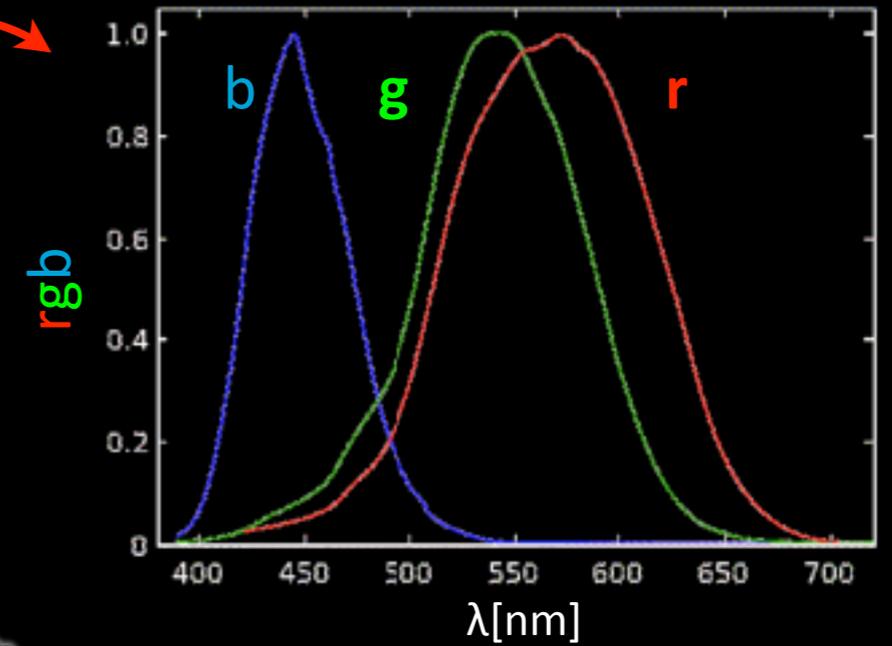
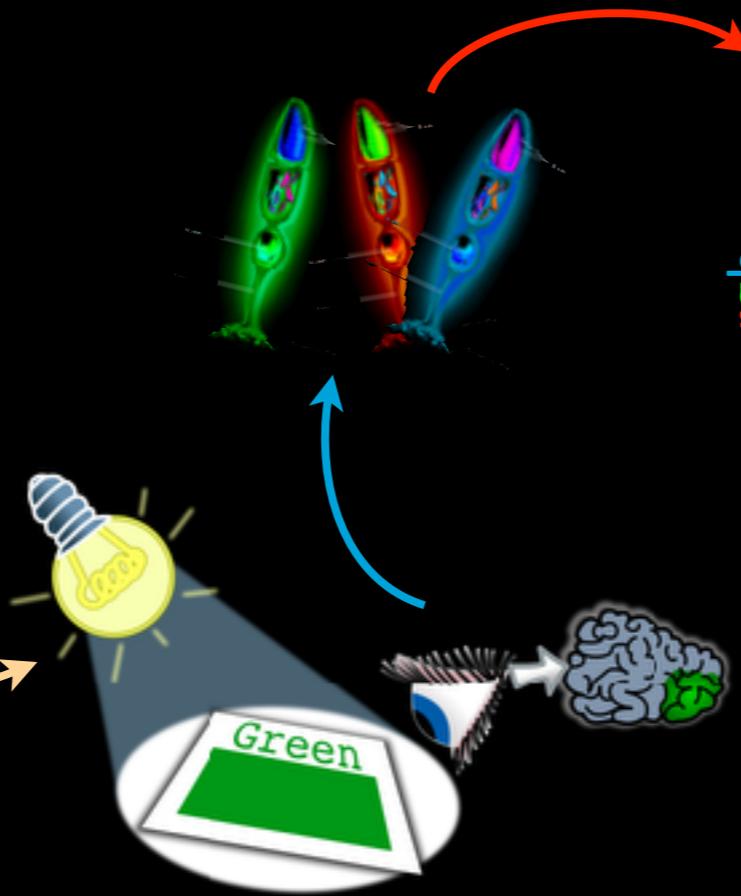
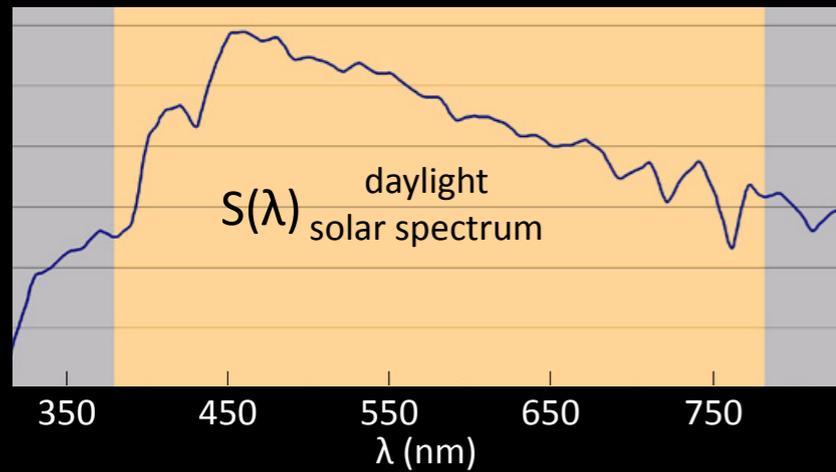


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$$RGB(x) = \int S(\lambda) e^{-\kappa(\lambda)x} rgb(\lambda) d\lambda$$

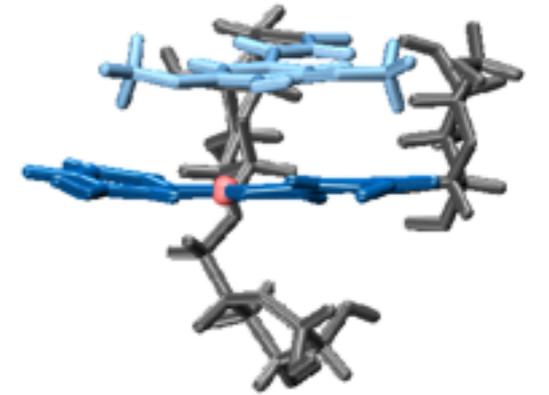


from chemistry to colour

chemical
composition

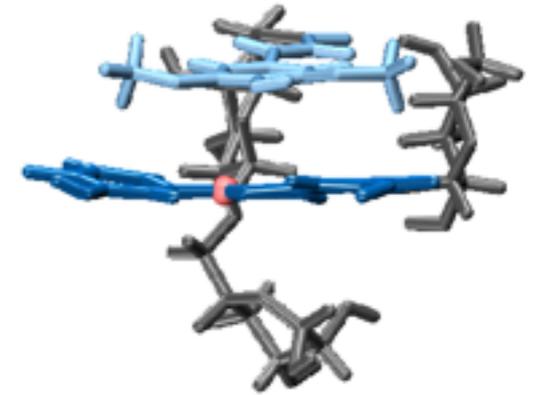
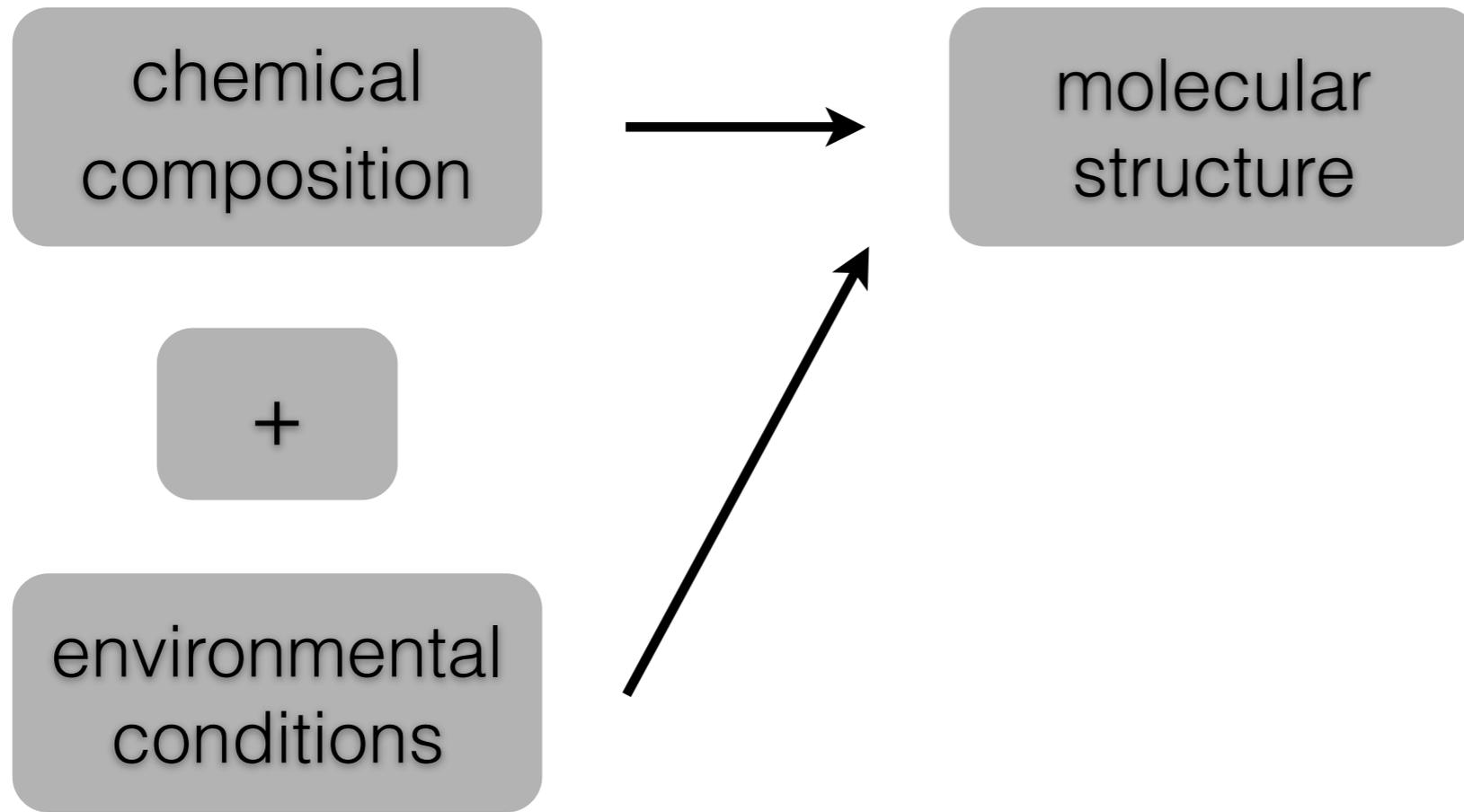


molecular
structure

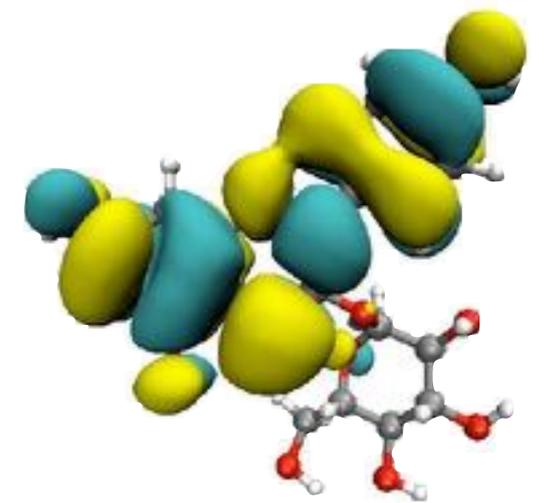
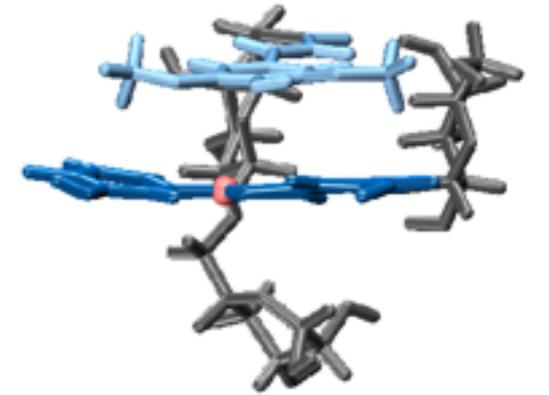
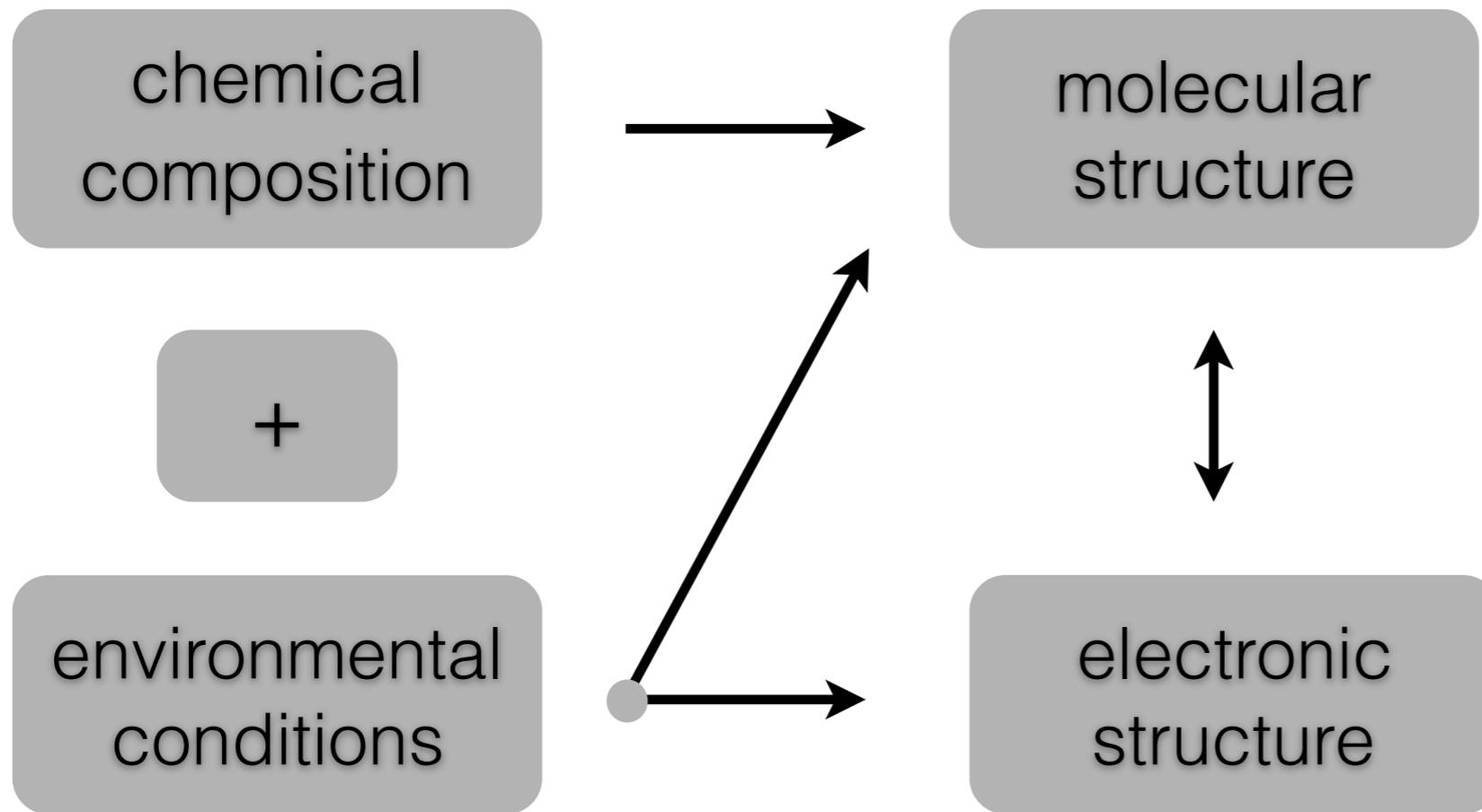


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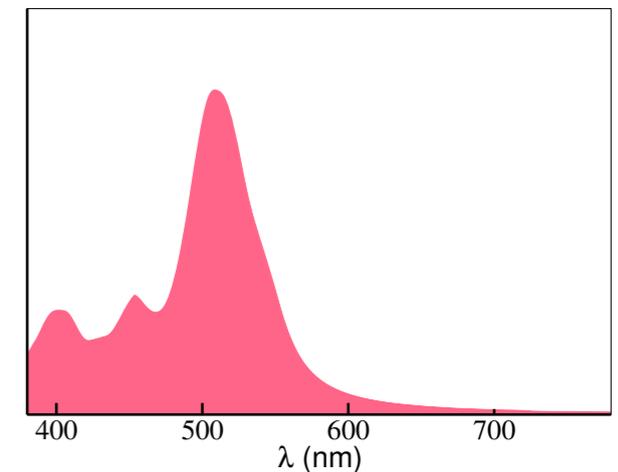
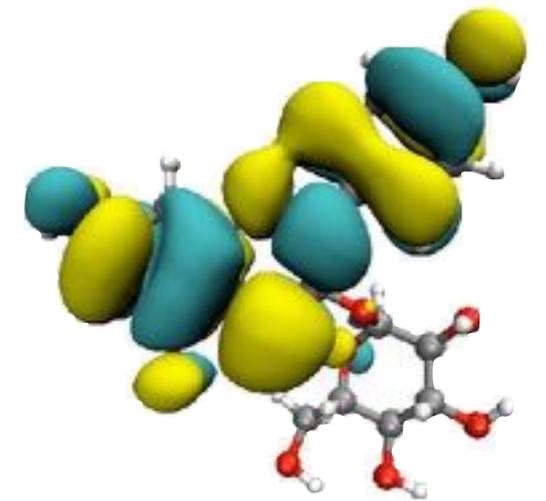
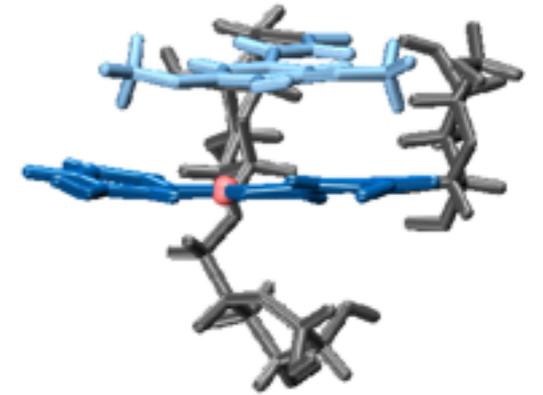
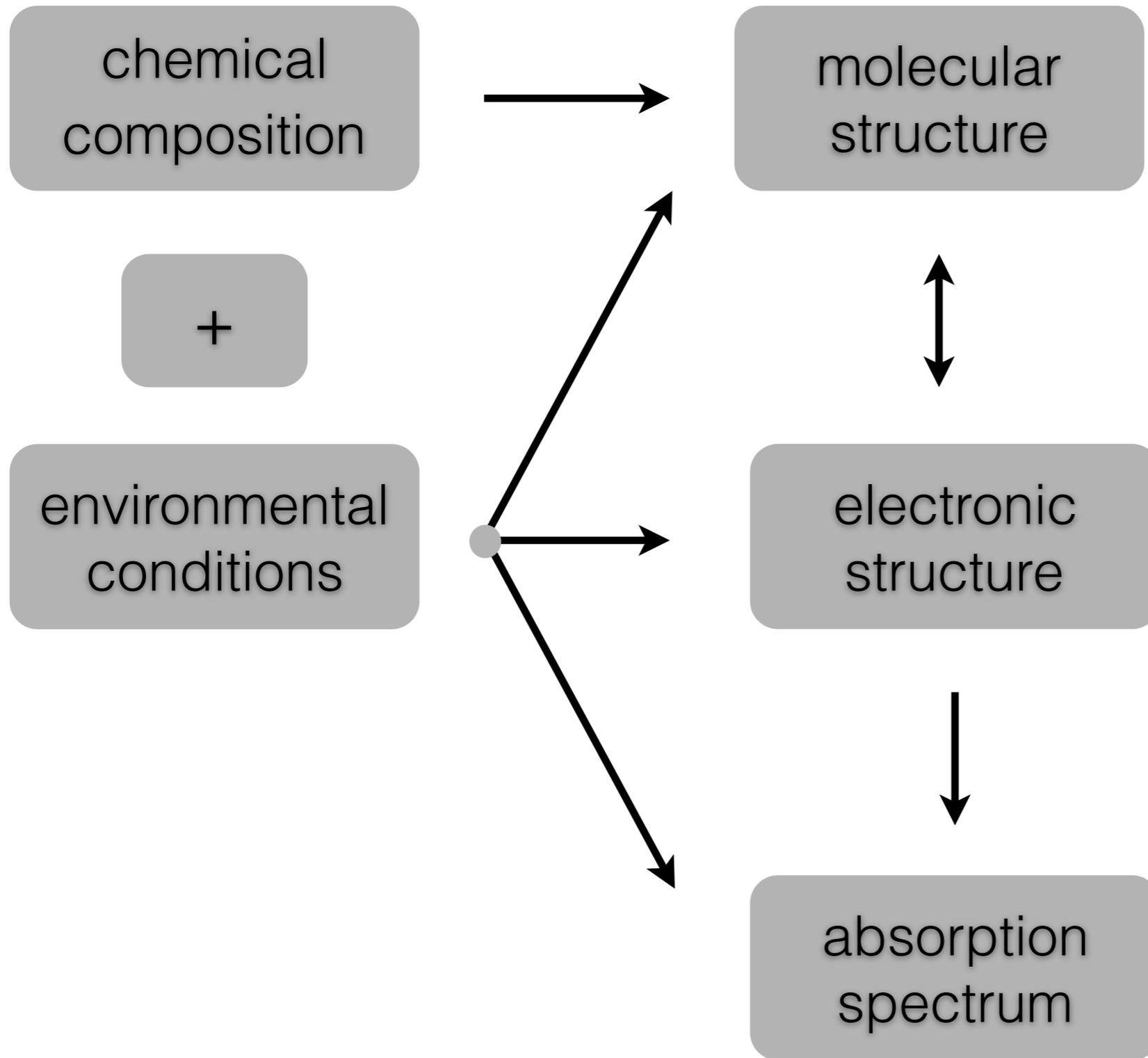
from chemistry to colour



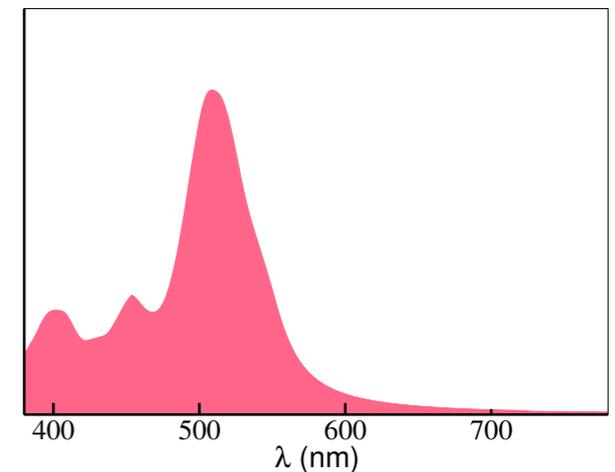
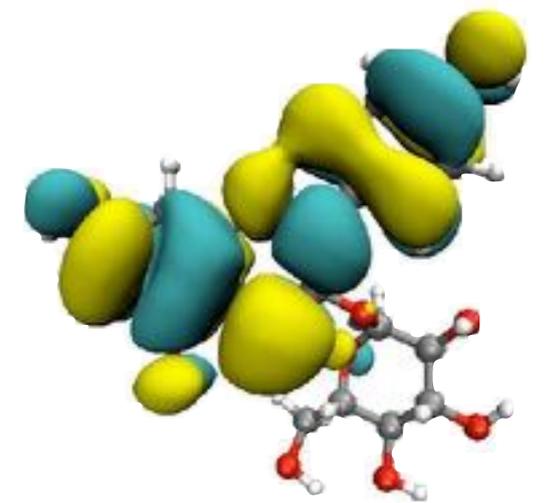
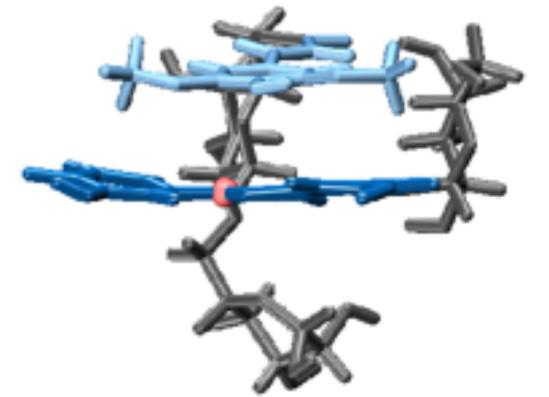
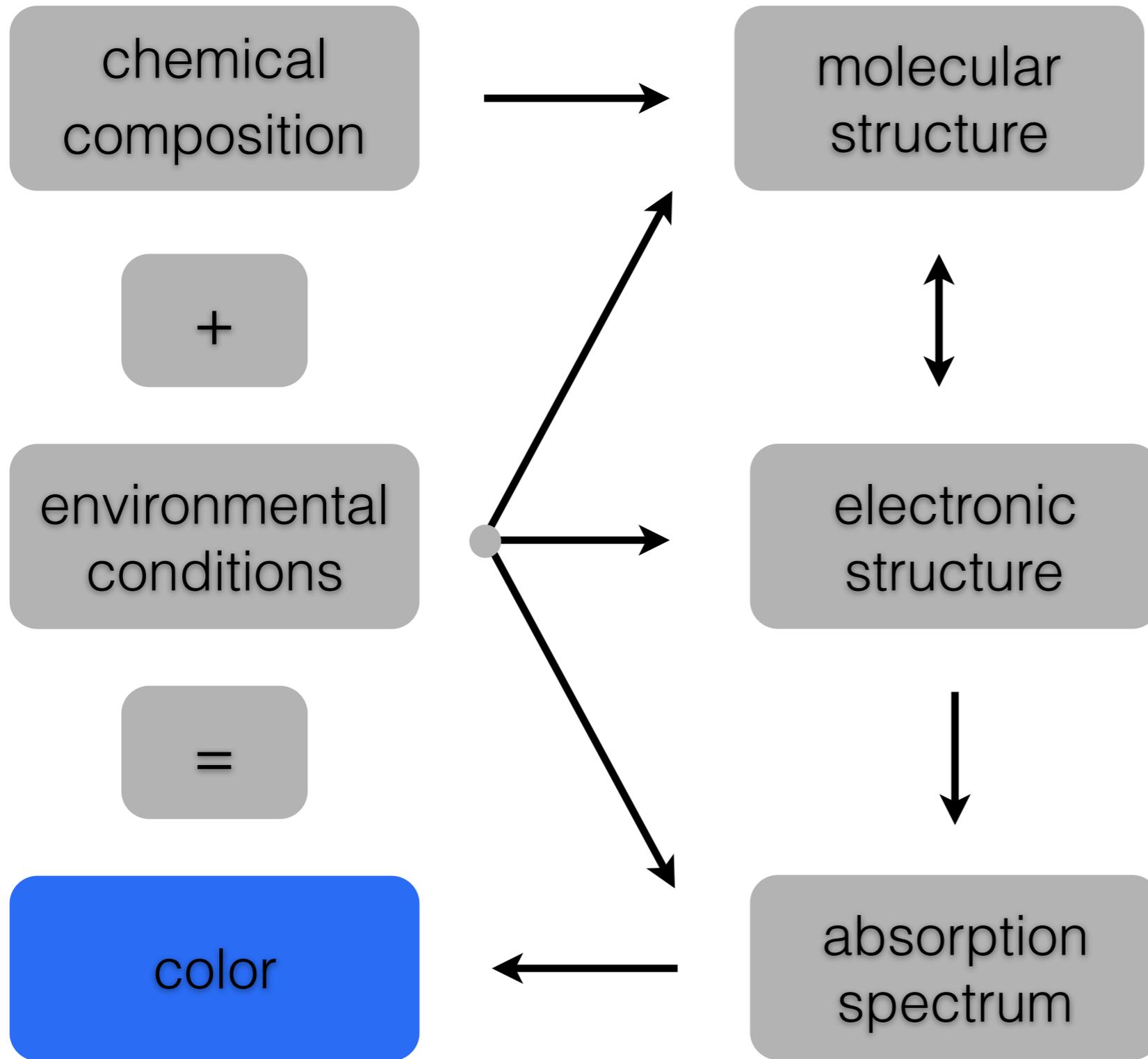
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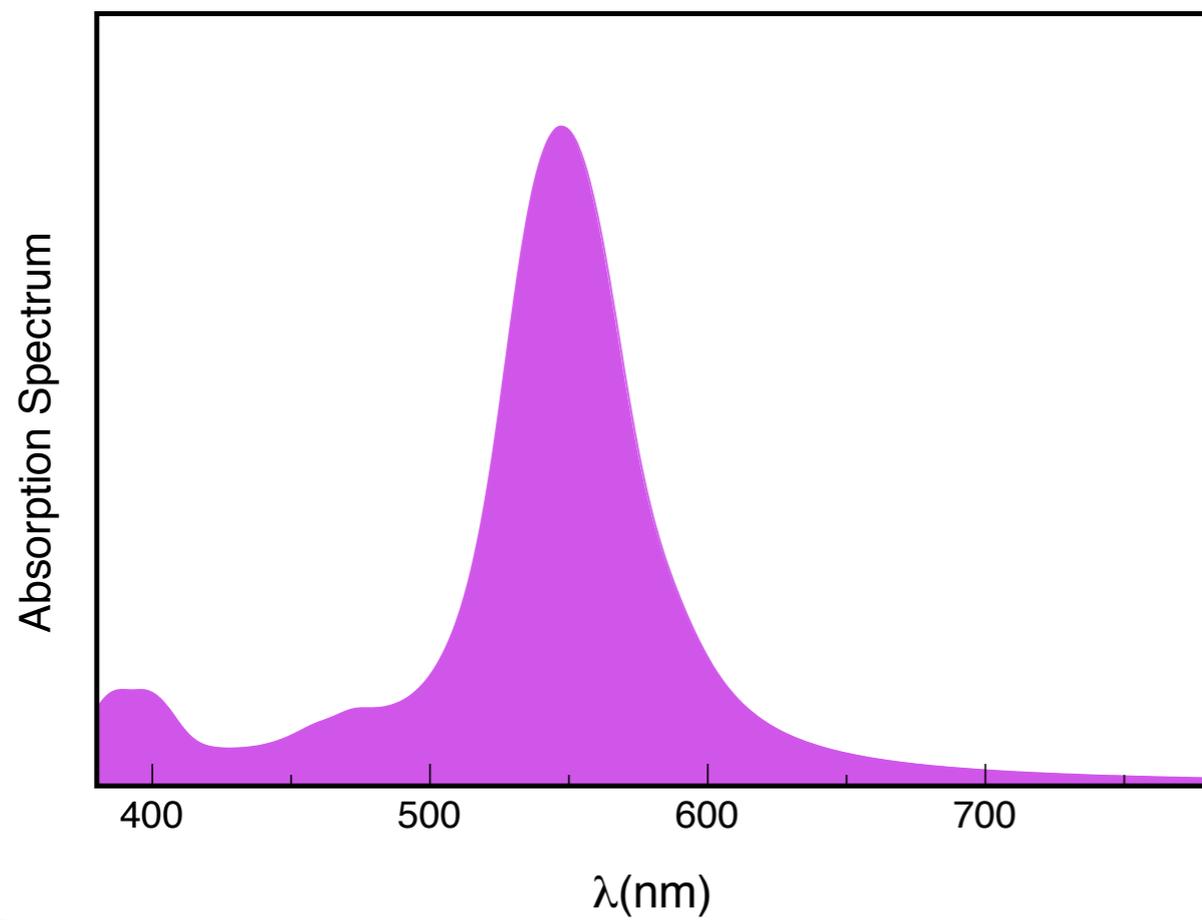
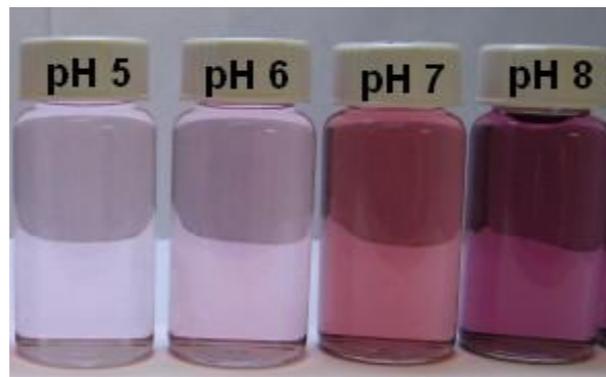
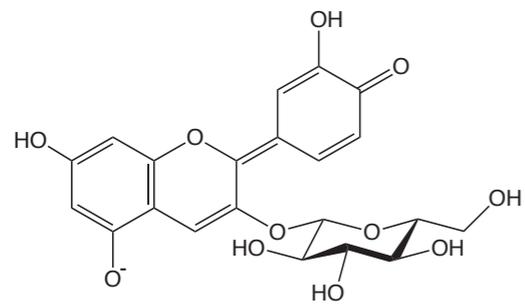


the multiscale protocol

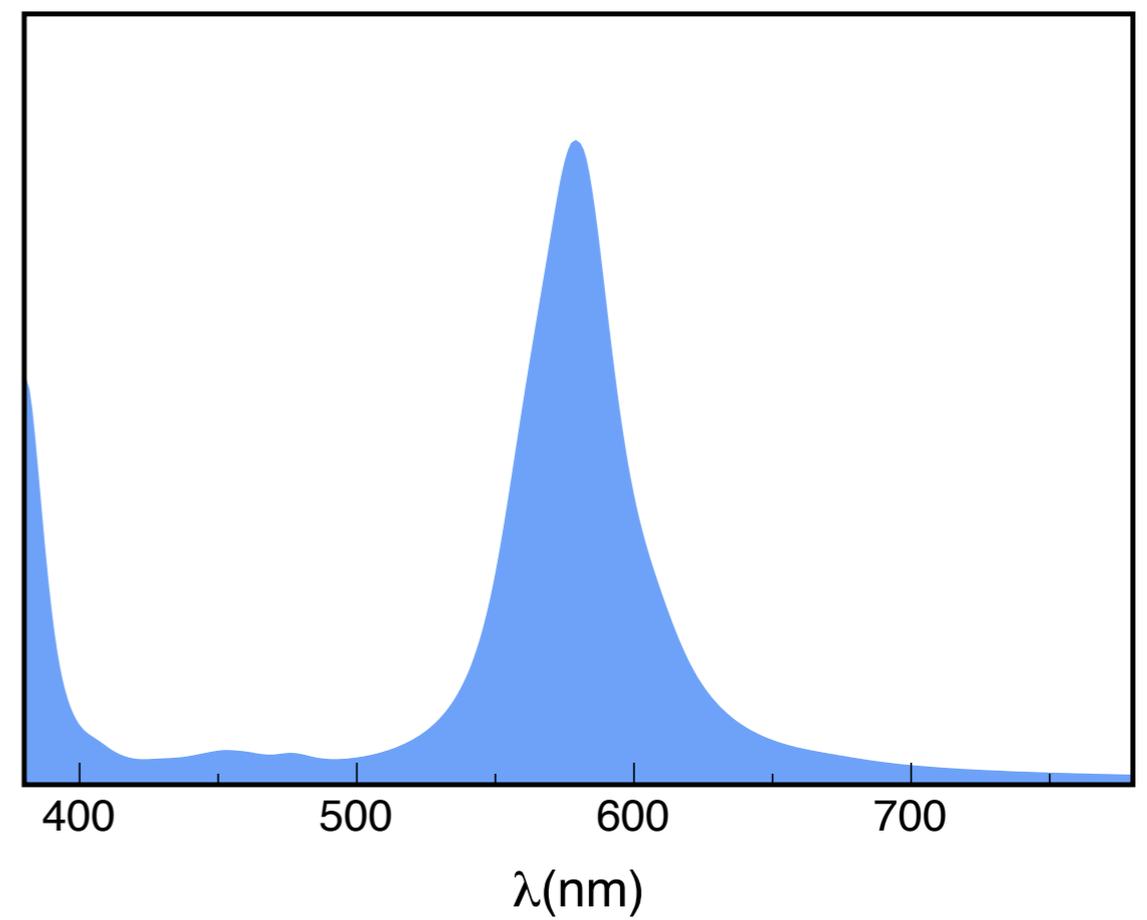
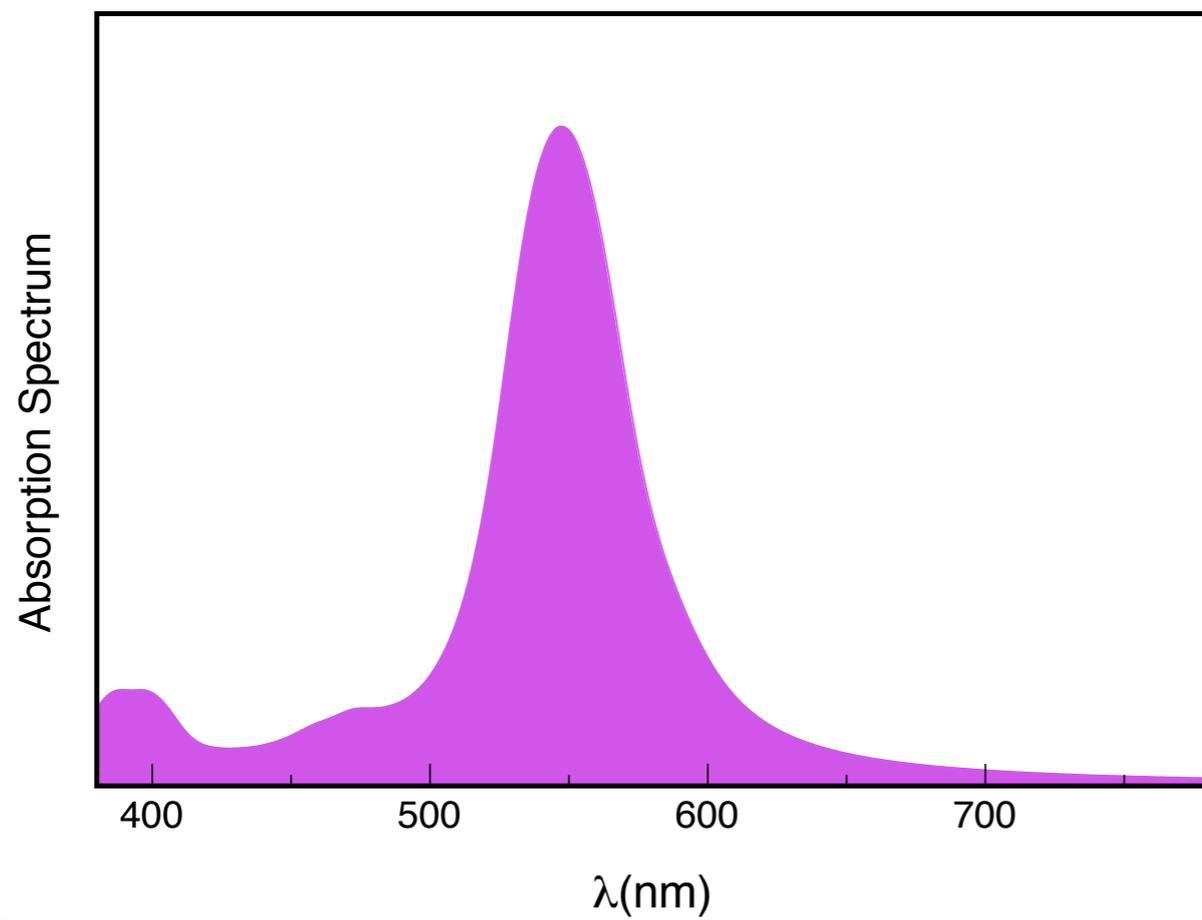
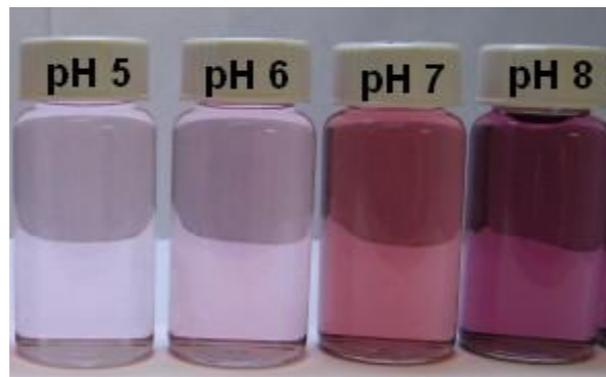
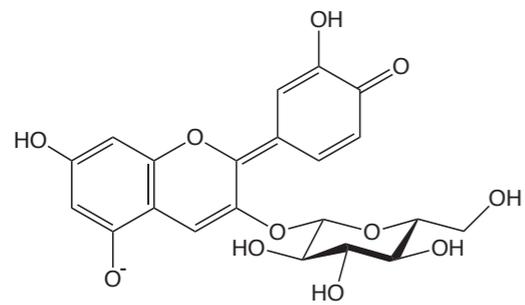
1. estimate conformational populations from **long ($> 1\mu\text{s}$) classical MD simulations** in explicit water solvent;
2. estimate quantum corrections to the classical populations from **thermodynamical perturbation theory**;
3. for each of the most populated molecular conformers thus identified, run a 10-20 ps **CPMD simulation**;
4. for each CPMD trajectory thus generated, compute **TDDFT spectra** on the fly $\approx 1\text{ps}$ apart, using a recently developed **self-consistent continuum solvation (SCCS) model**;
5. **average** the spectra thus generated for each conformer;
6. **average** the spectra over different conformers, weighing with the populations computed in 1-2.



in the quest for a natural *blue 2*



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$$-\frac{\hbar^2}{2m} \Delta \psi_n(x) + V(x) \psi_n(x) = E_n \psi_n(x)$$



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<https://talks.baroni.me>