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quantum mechanics on the supermarket shelf

how theoretical physics helped design a healthier colorant for popular candies

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Trieste — Italy

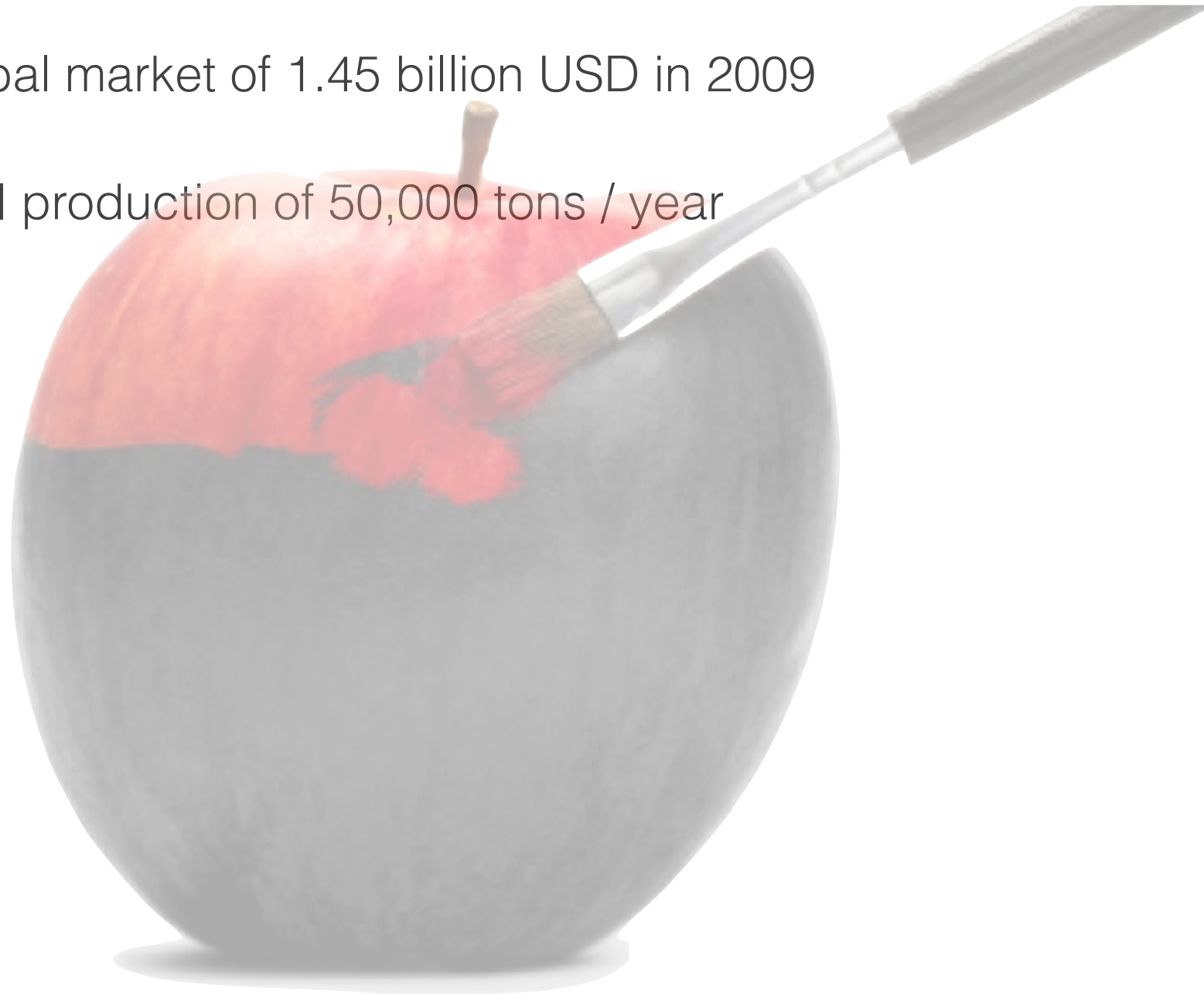
natural dyes in the food industry



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👉 global market of 1.45 billion USD in 2009

👉 total production of 50,000 tons / year



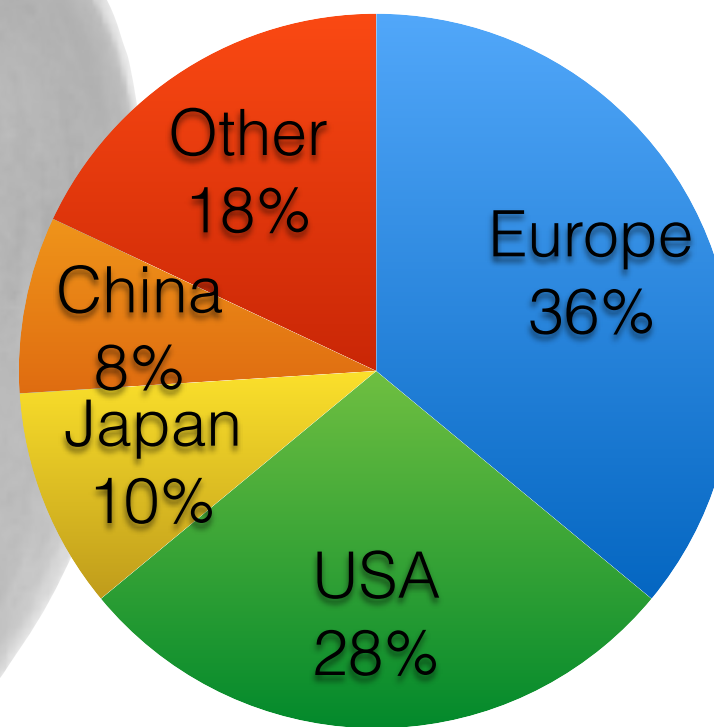
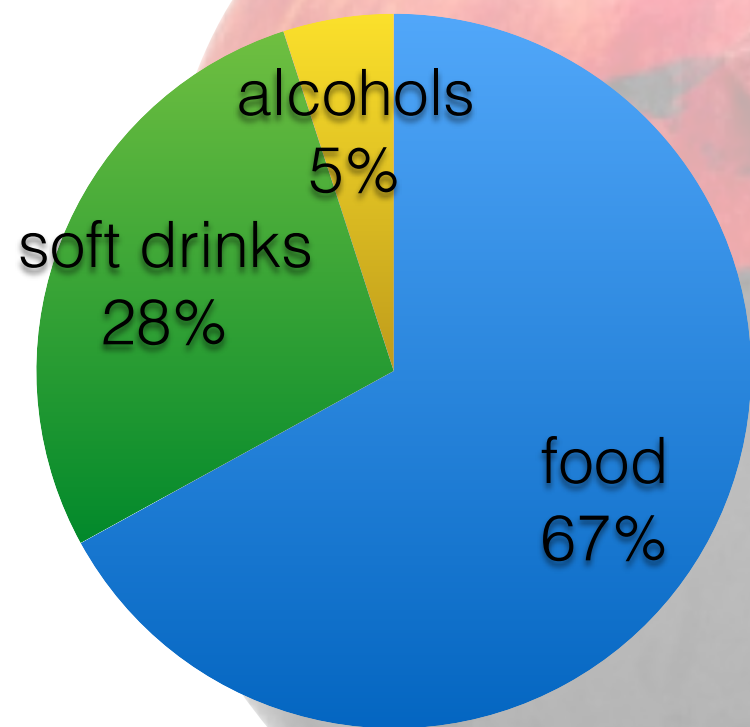
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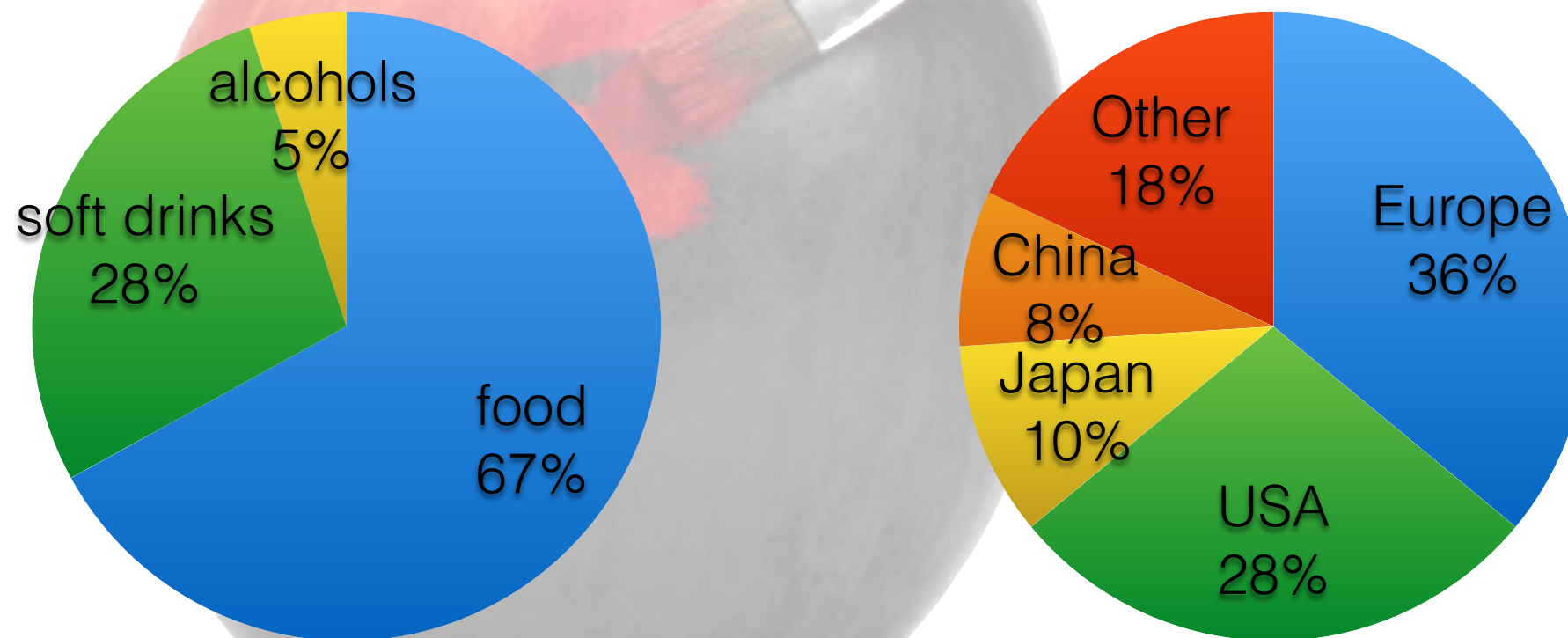
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👉 natural dyes market grown by 35% in the 2005-2009 quinquennium

natural dyes: the requirements

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 tunable

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- tunable

- stable

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- safe

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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*



MAX

the Southampton six

In 2007 Research funded by the UK FSA was published, suggesting that consumption of mixes of certain artificial food colours and the preservative sodium benzoate 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:



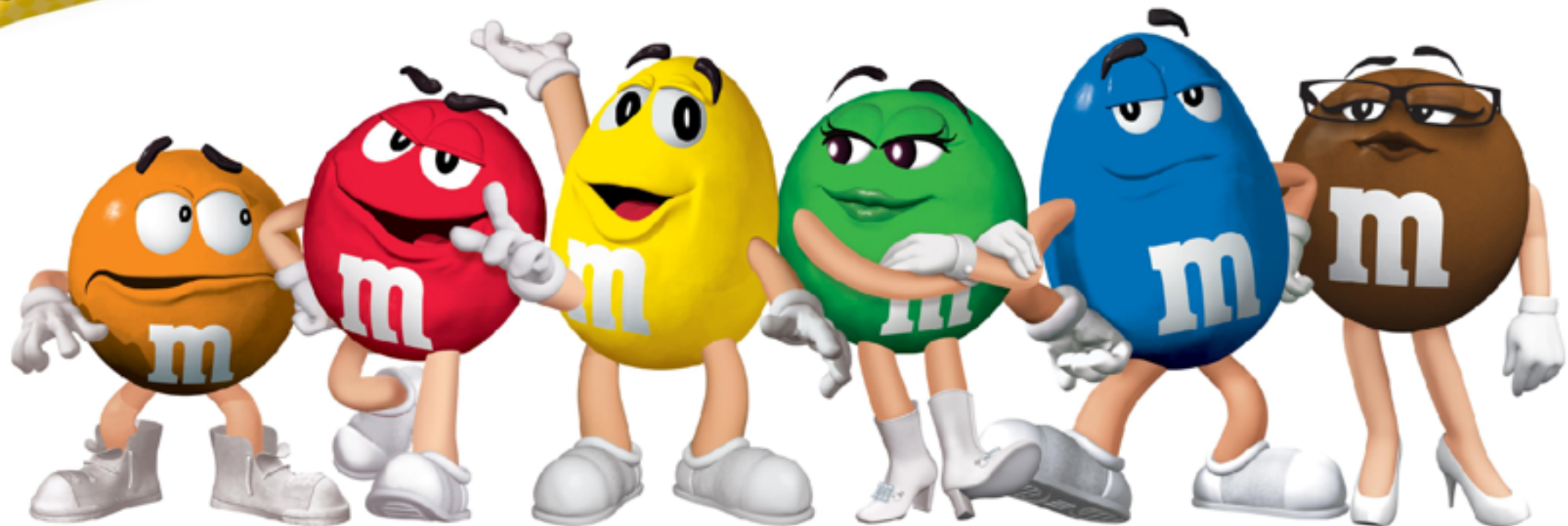
Sodium benzoate (E211)

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”

MARS

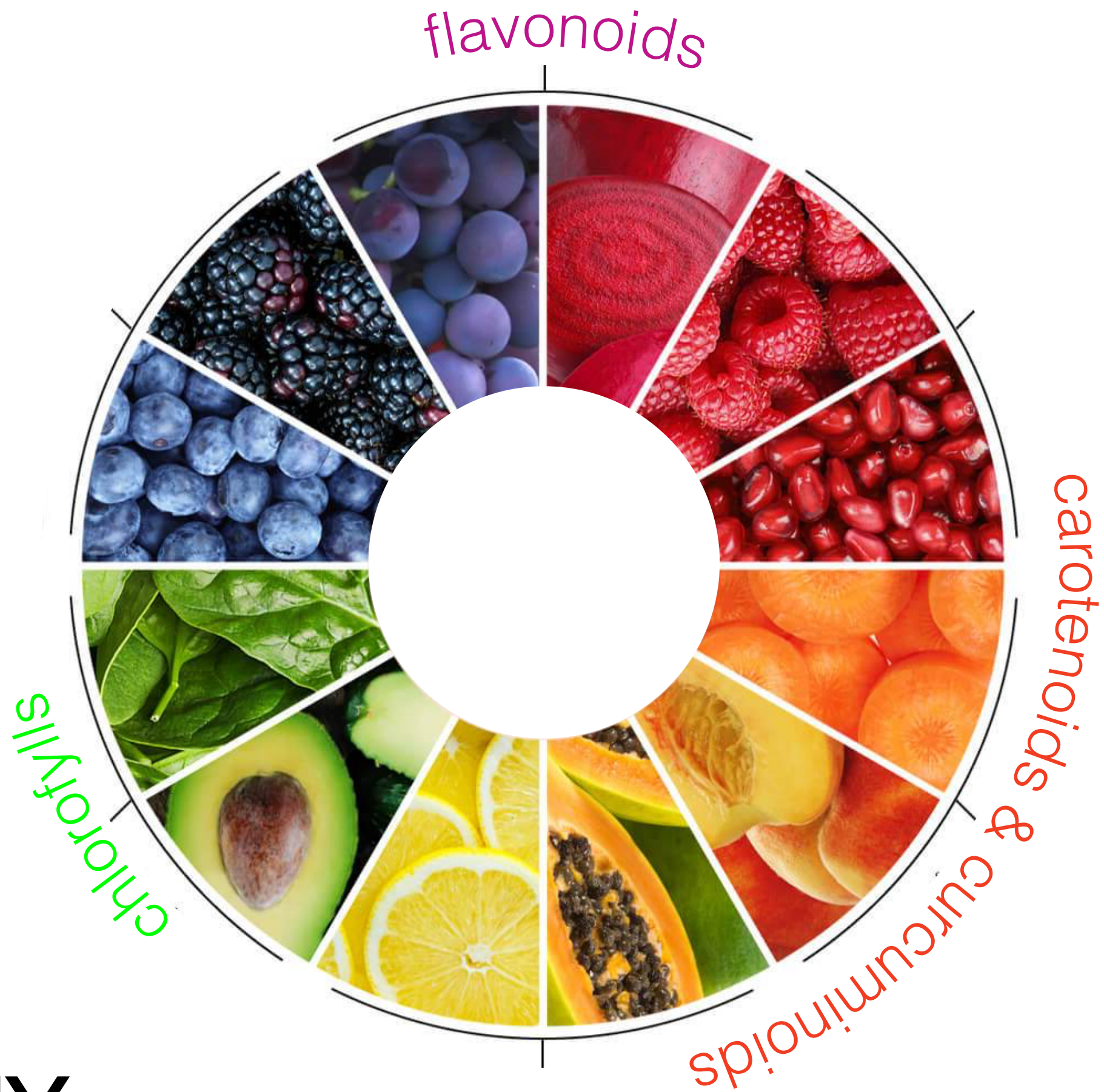
chocolate
north america

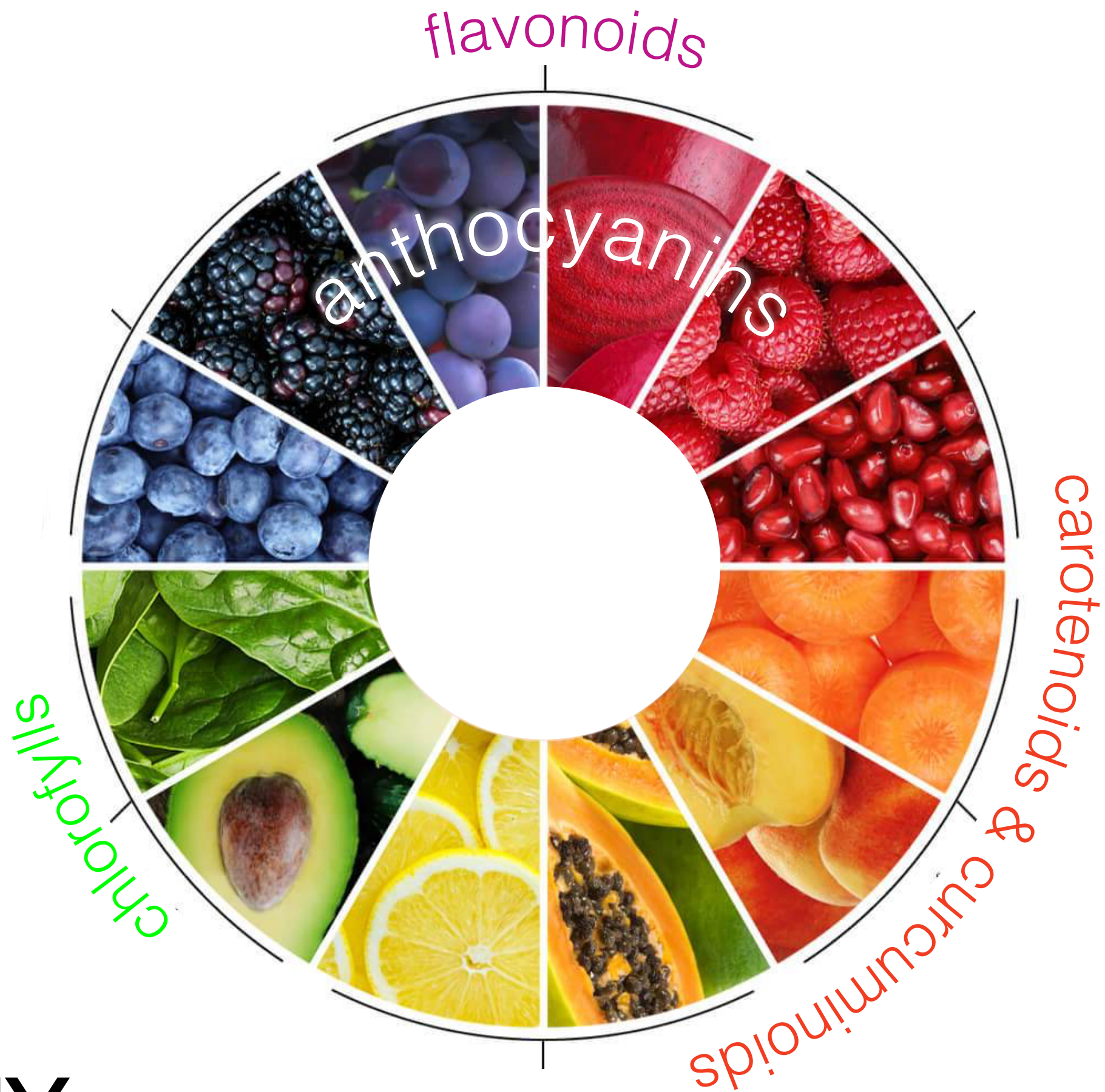


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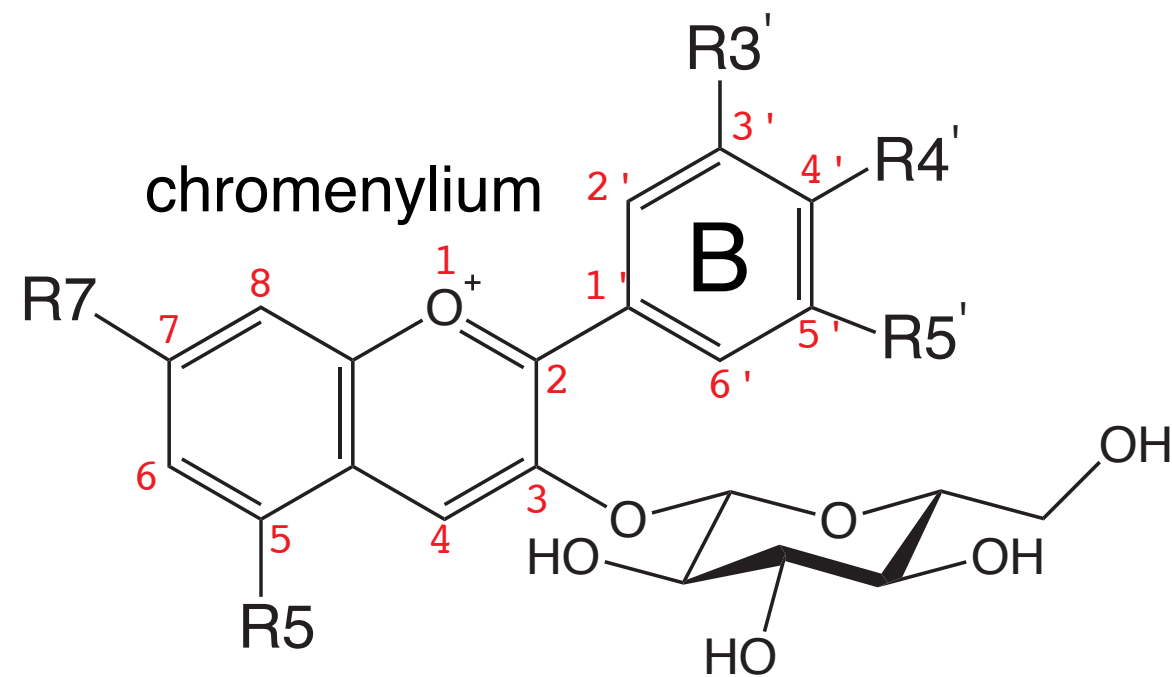
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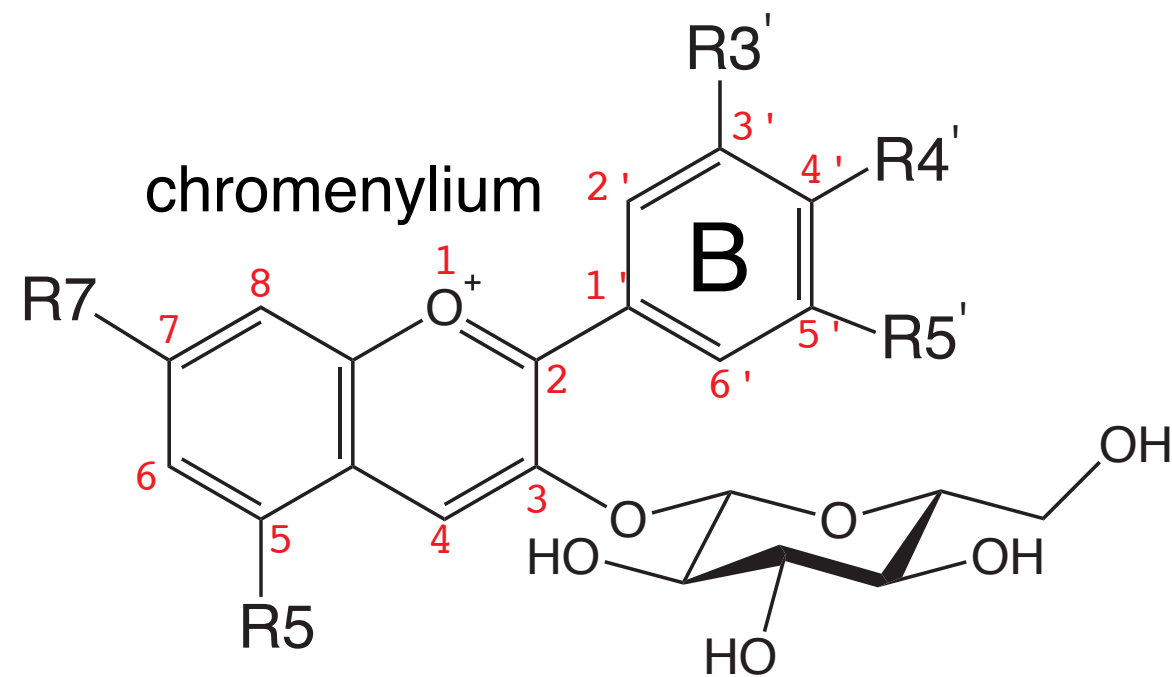
anthocyanins



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



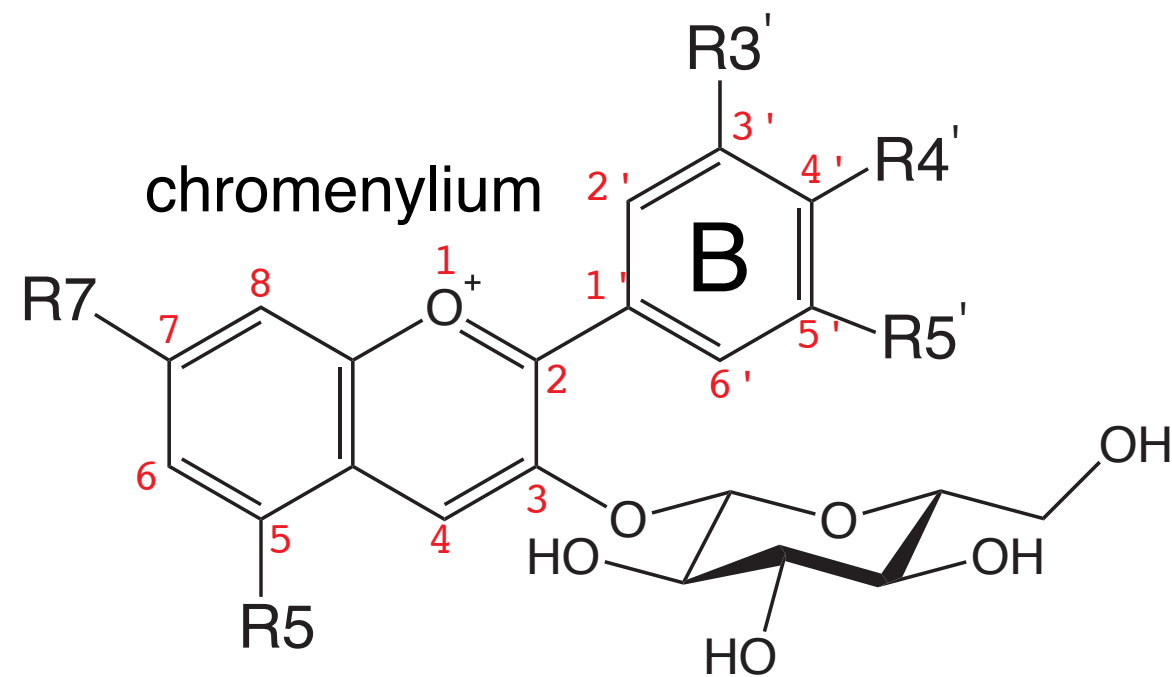
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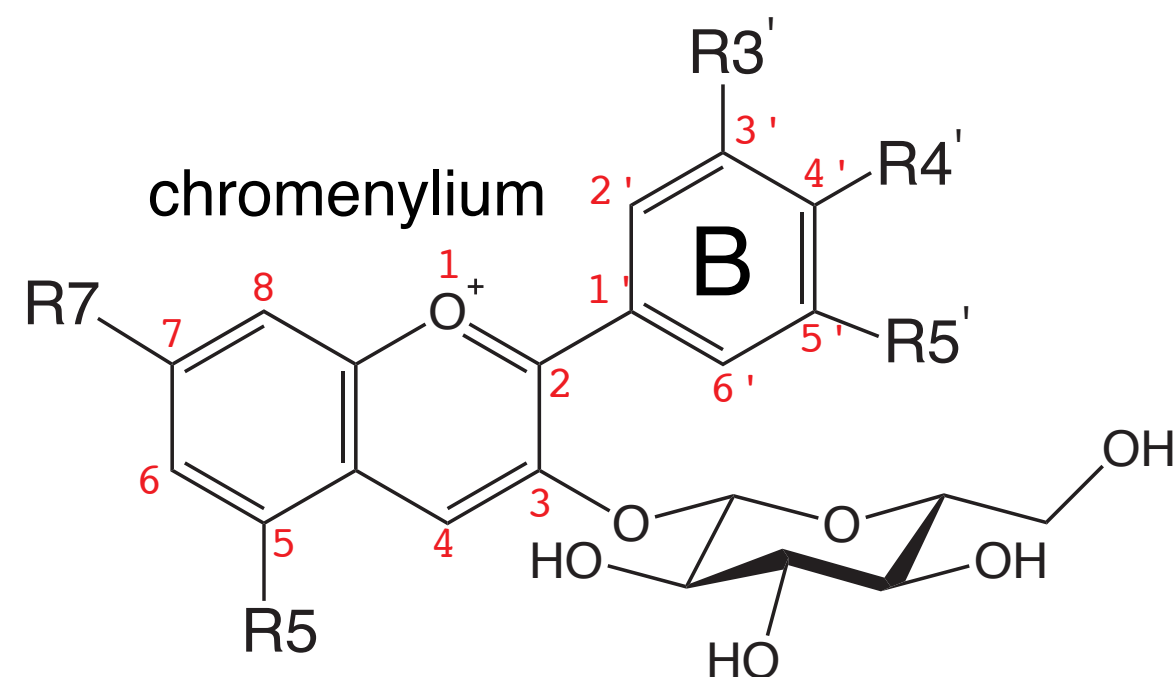
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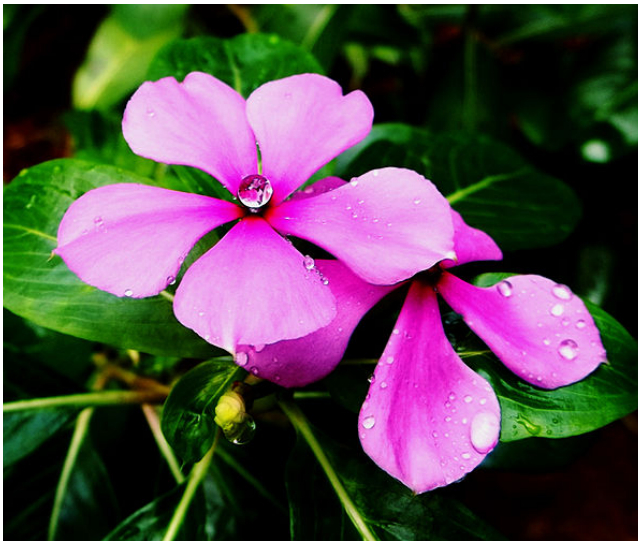
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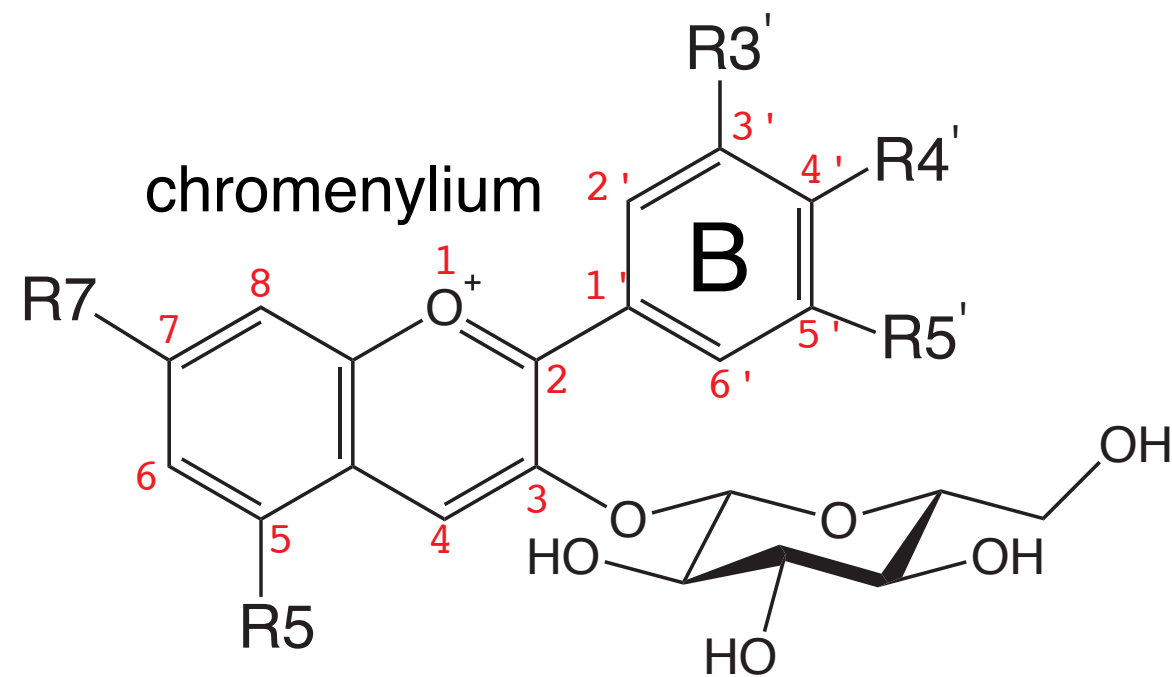
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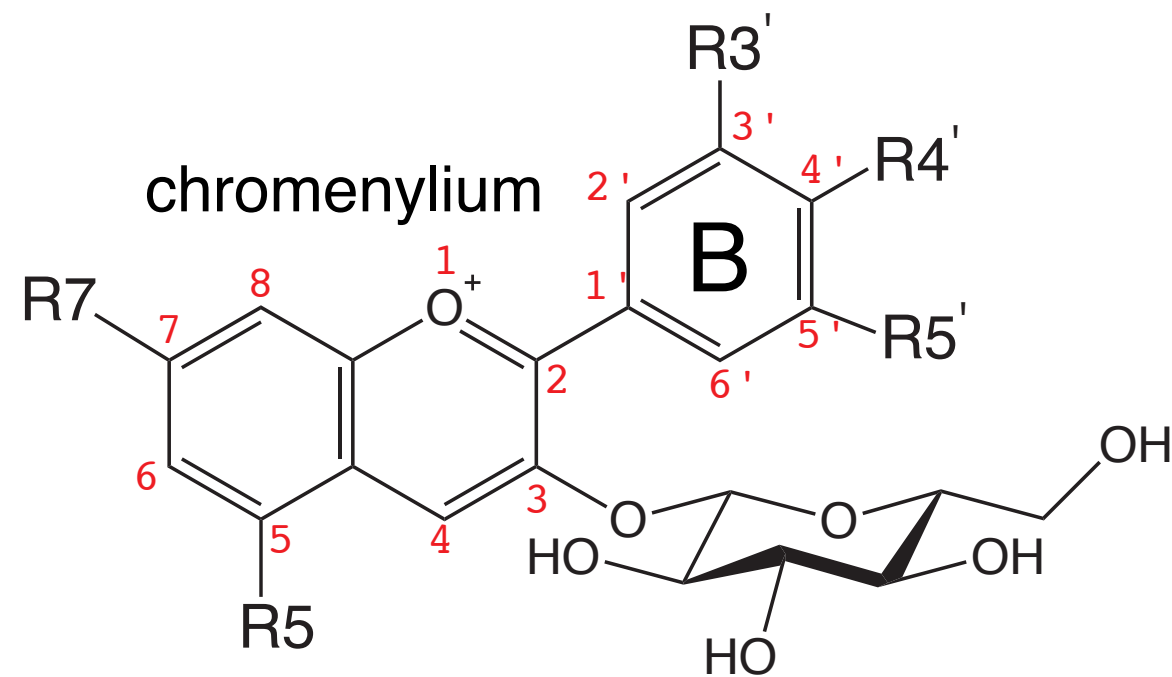
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pelargonin	-H	-OH	-OH	-OH



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;

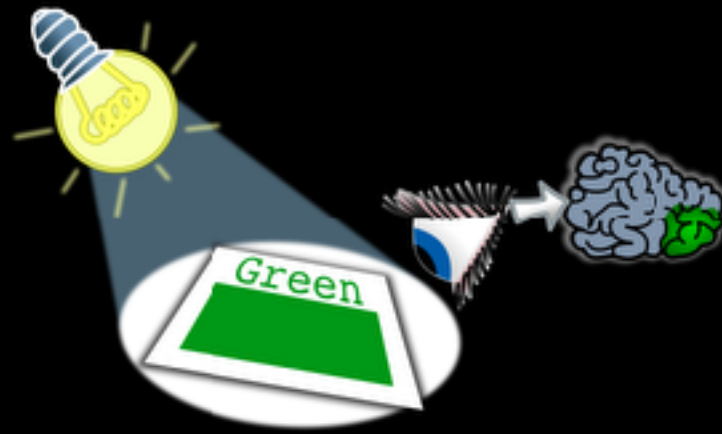
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 - very little research is being done in this area;
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 - most of it simply aims at isolating from natural sources (highly expensive and difficult);
- very little is known of the microscopic mechanisms that determine the stability and the chromatic properties of anthocyanins and the relation between structure and color.

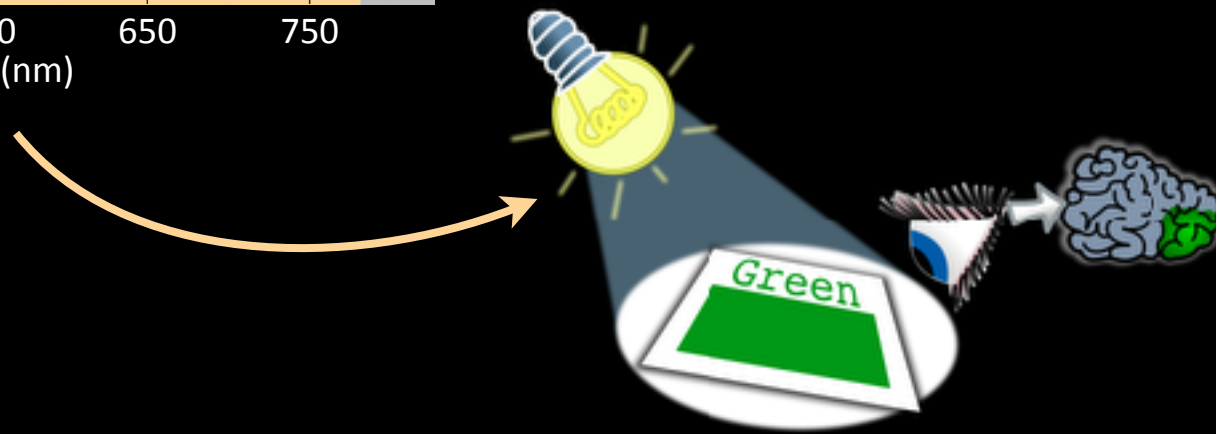
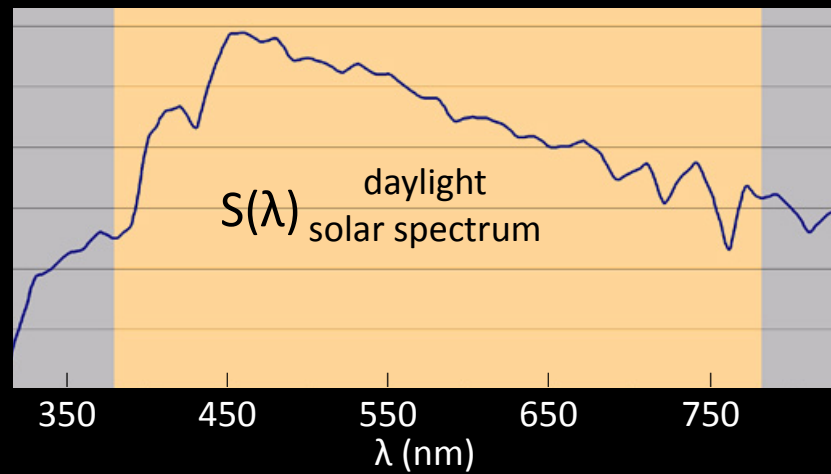
what color is all about



stimulus =

illuminant × transmission × sensitivity

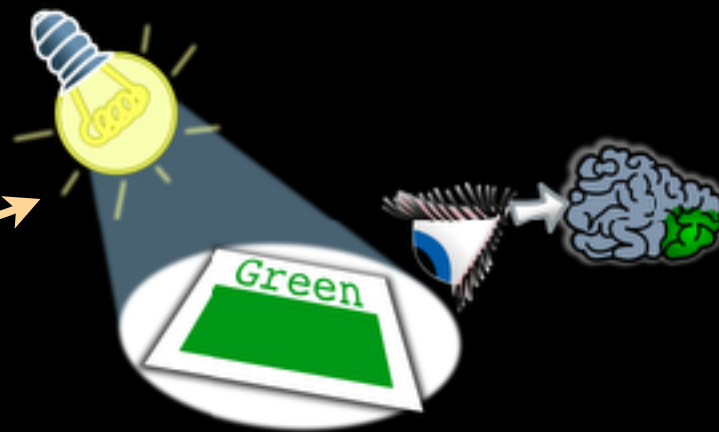
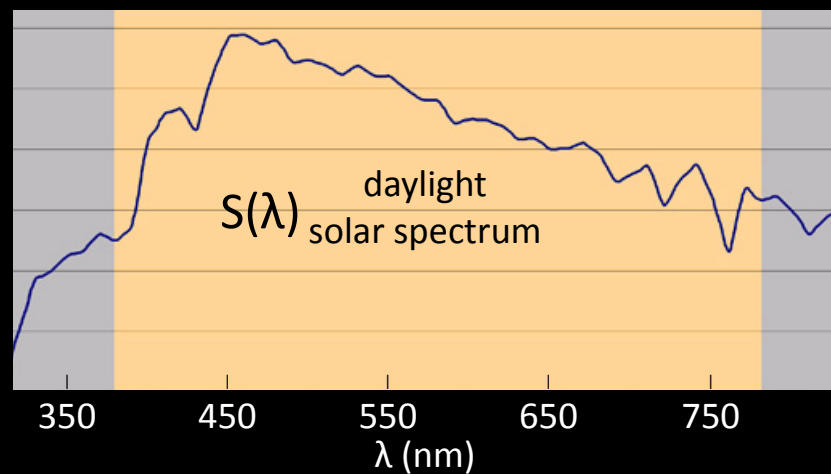
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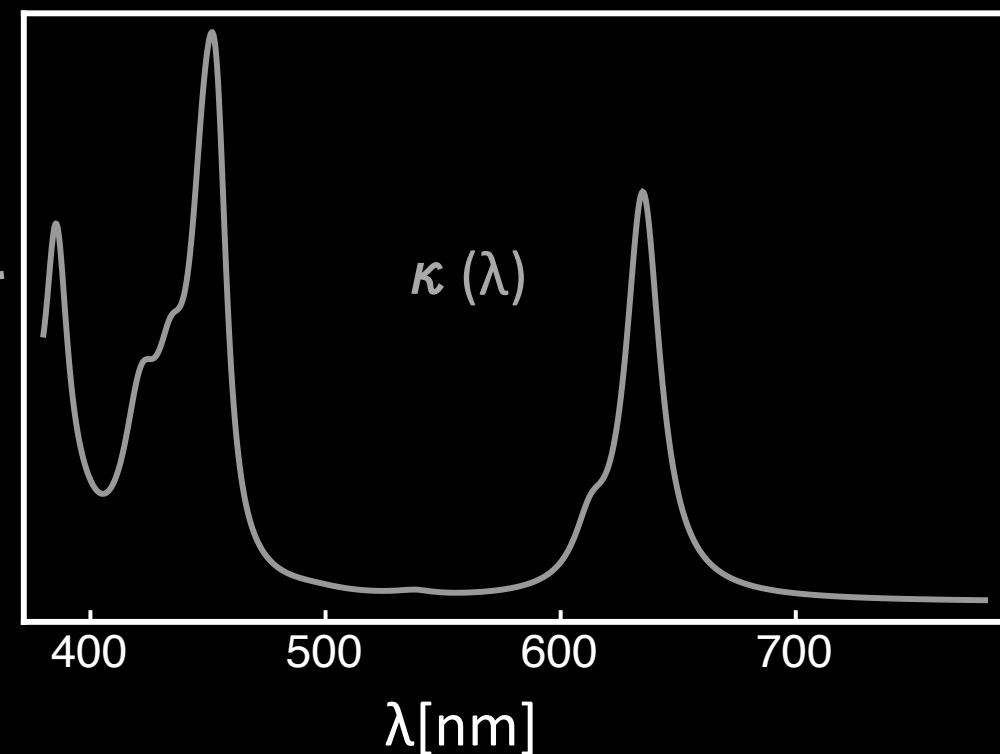
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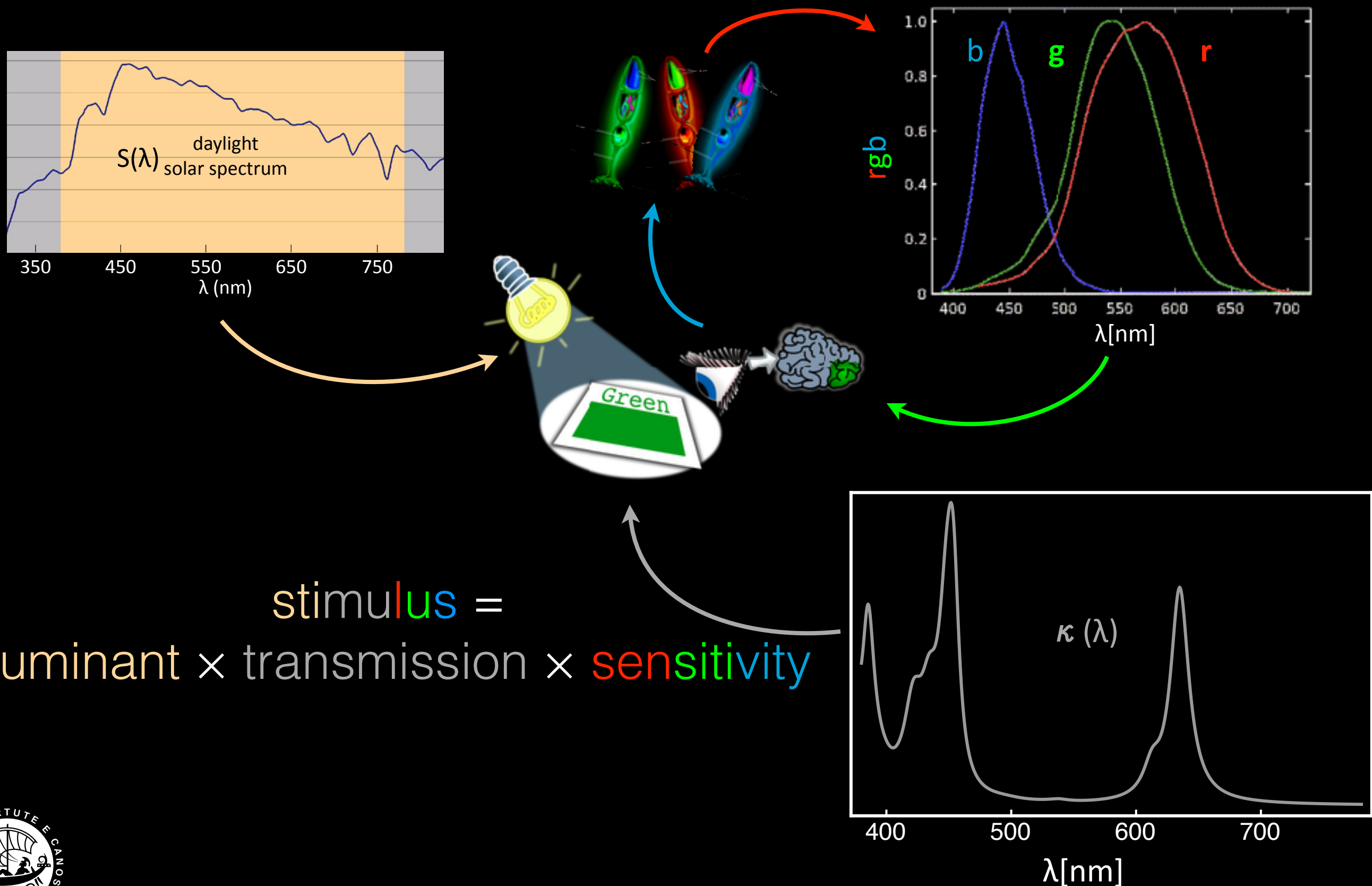
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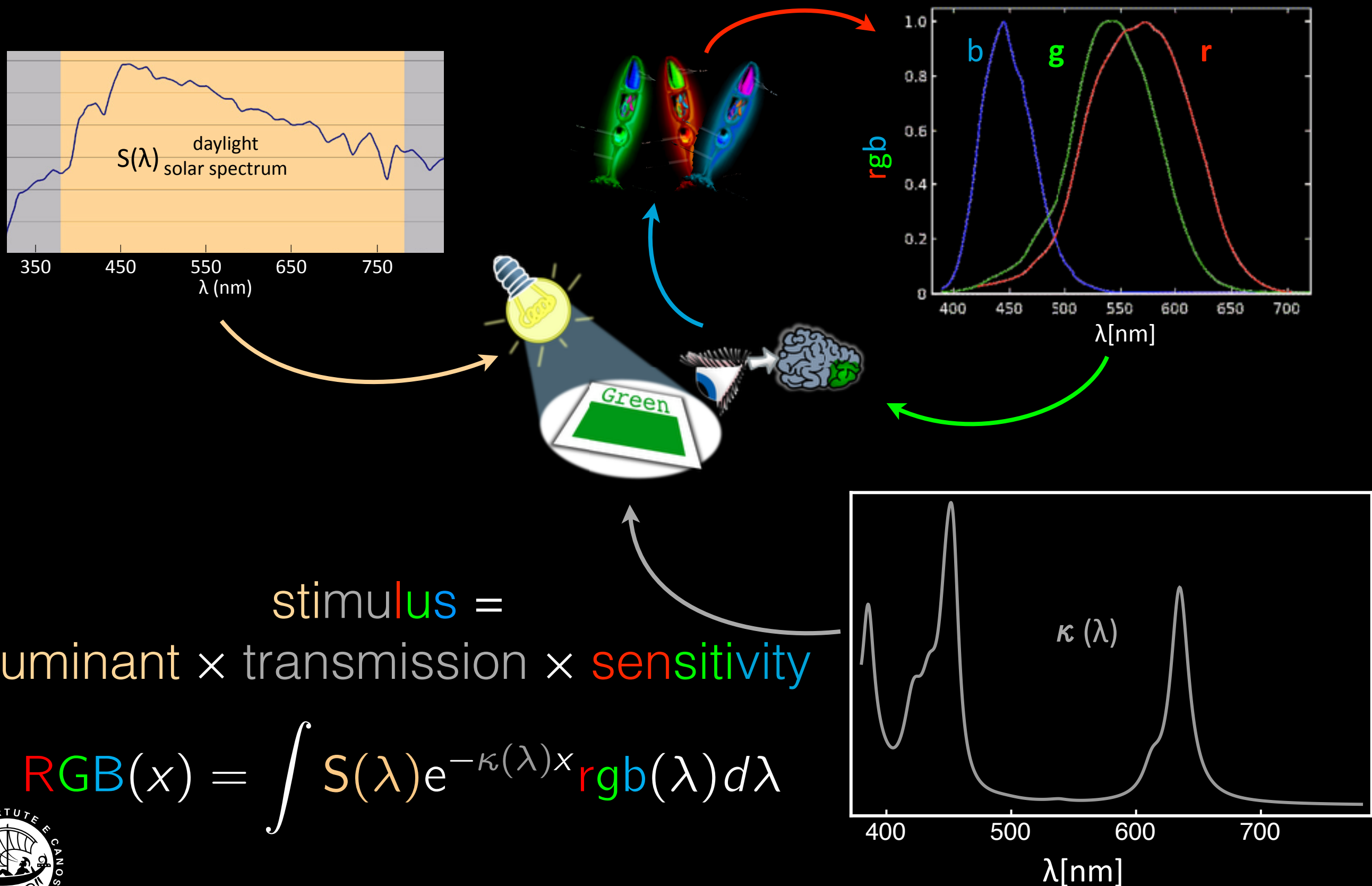
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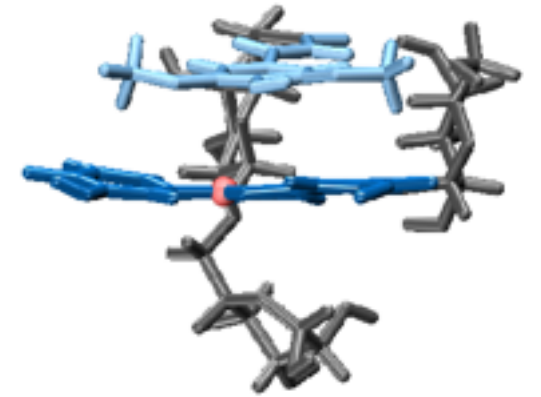


from chemistry to colour

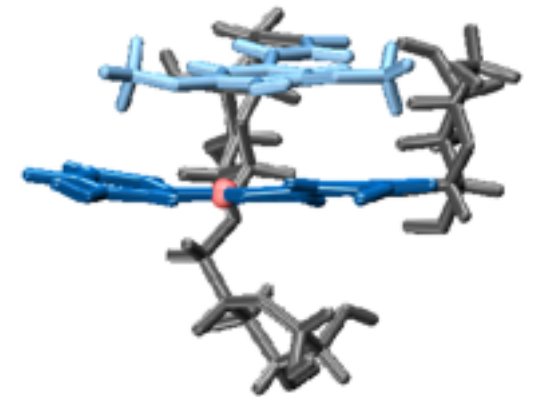
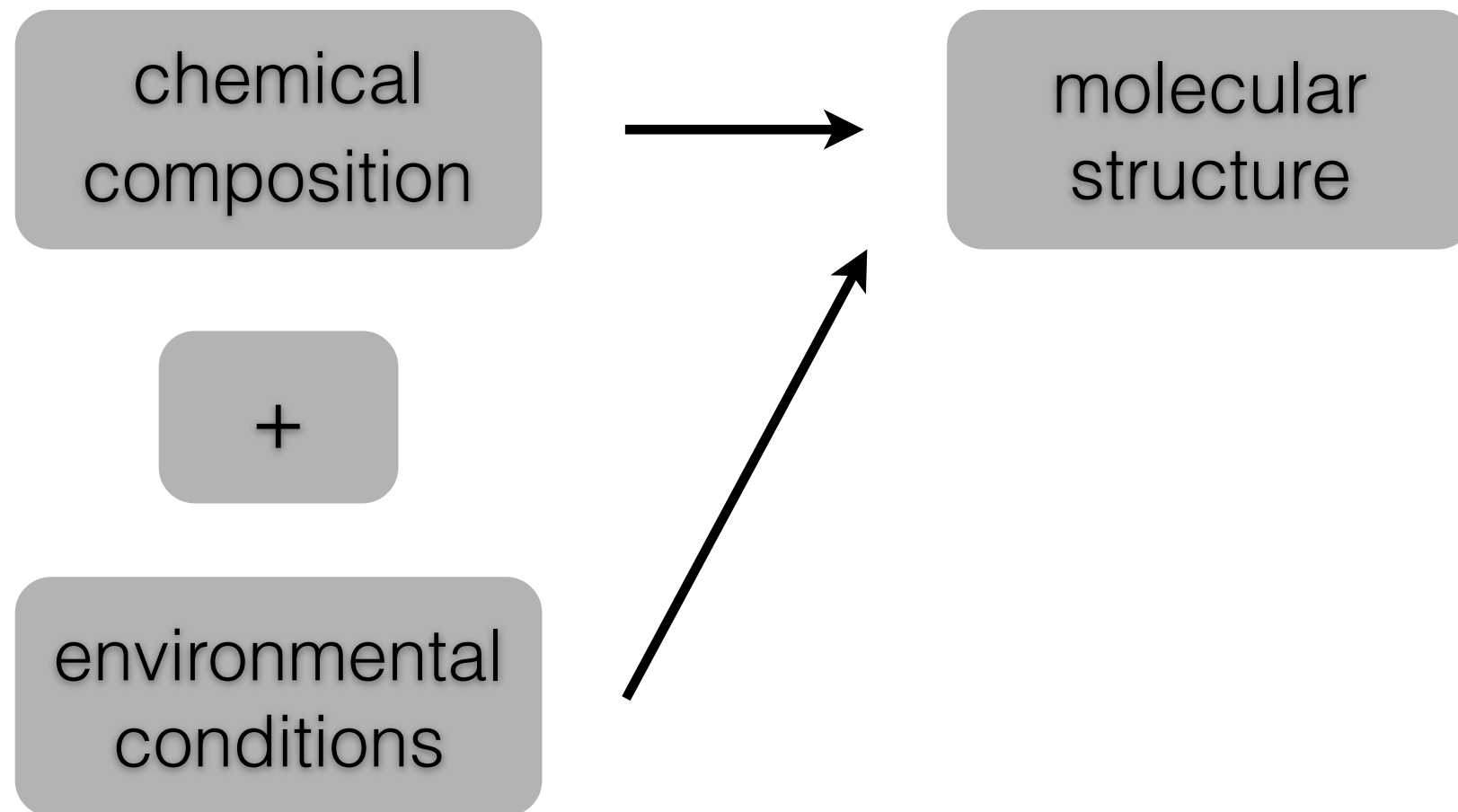
chemical
composition



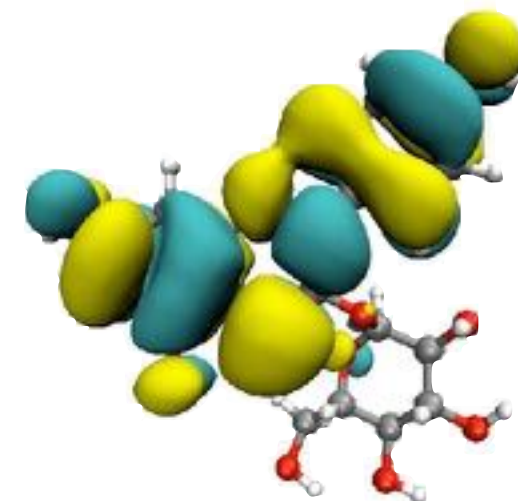
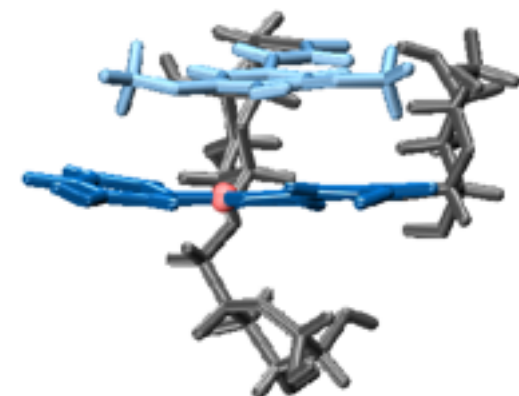
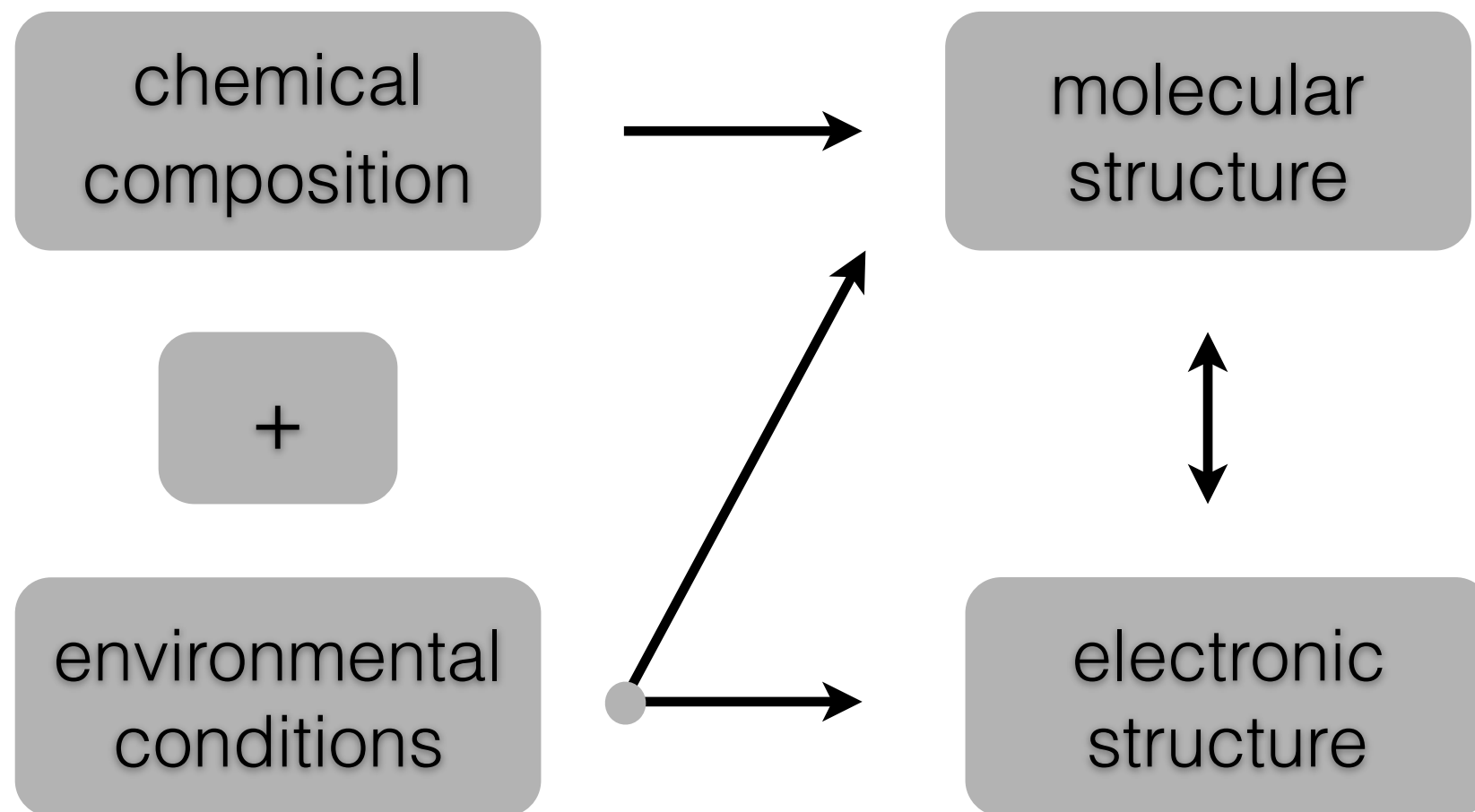
molecular
structure



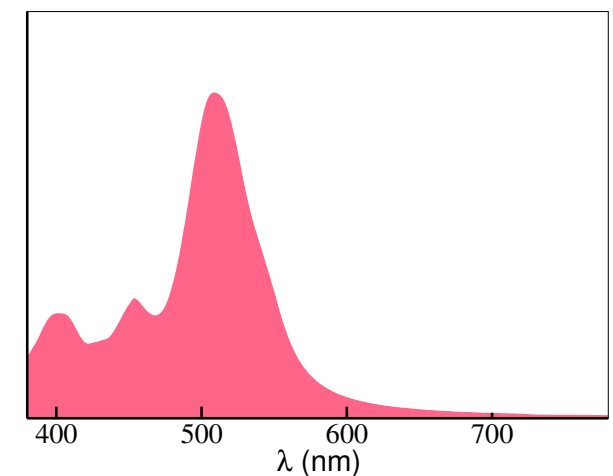
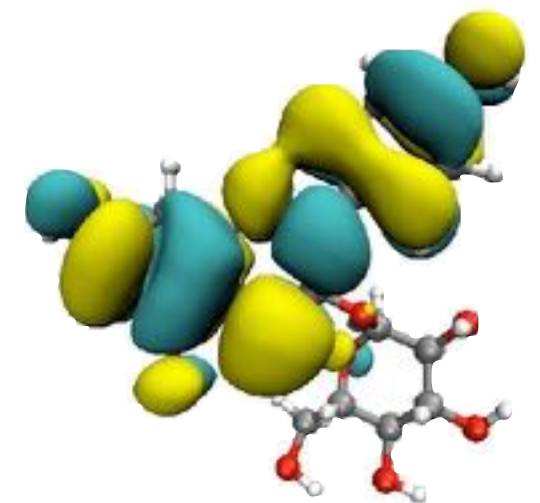
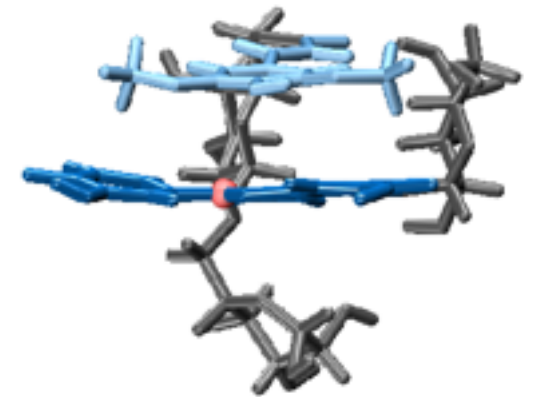
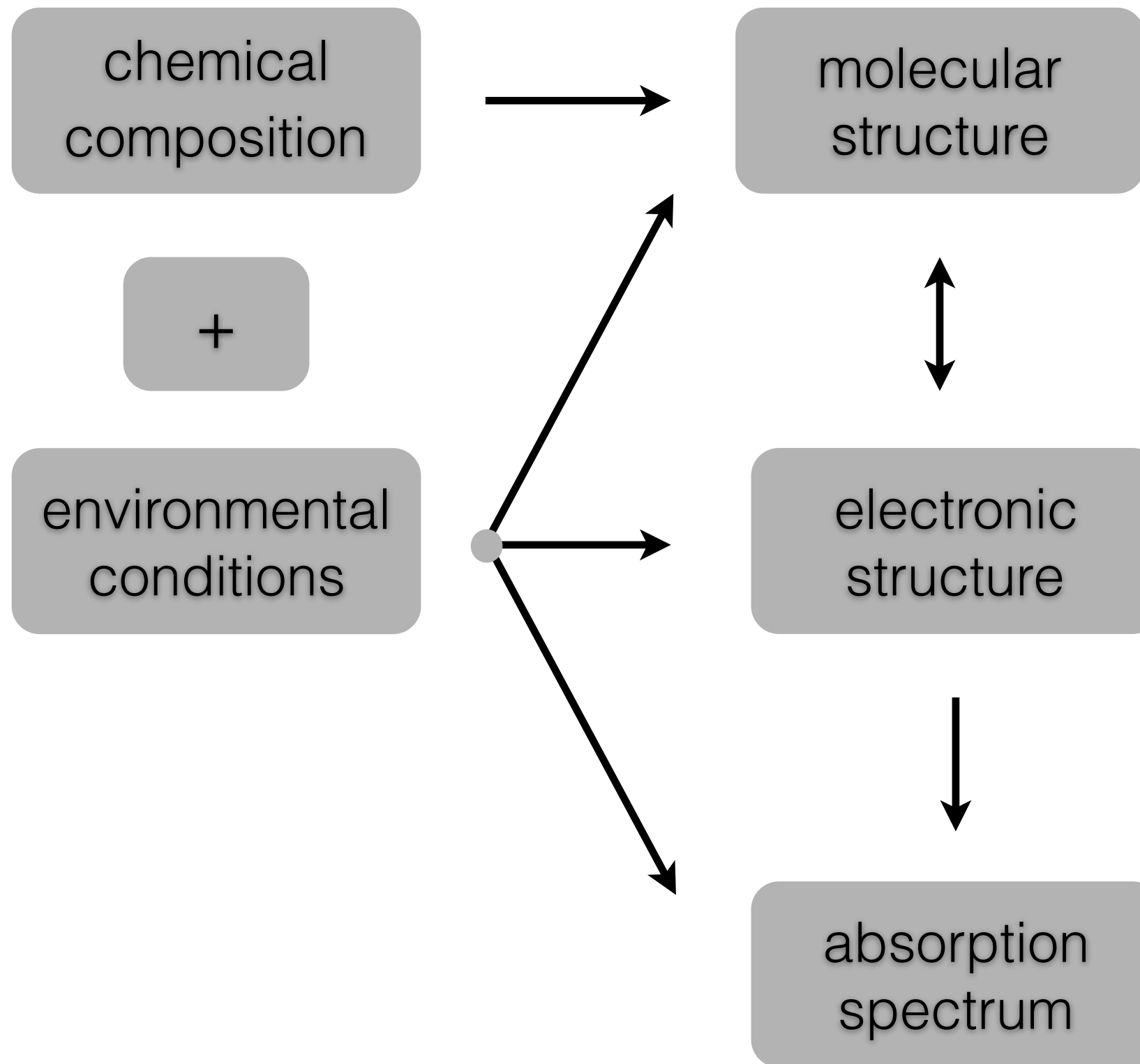
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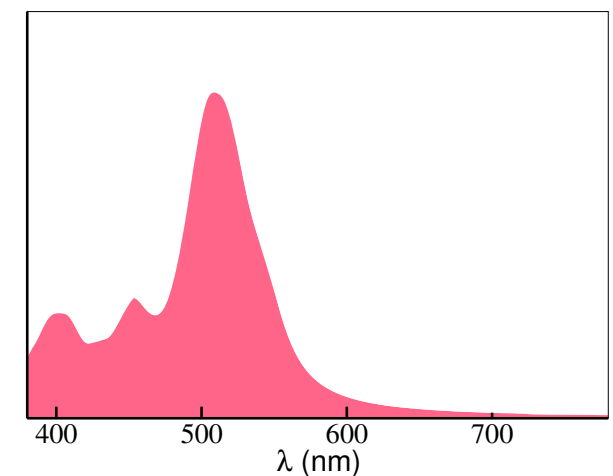
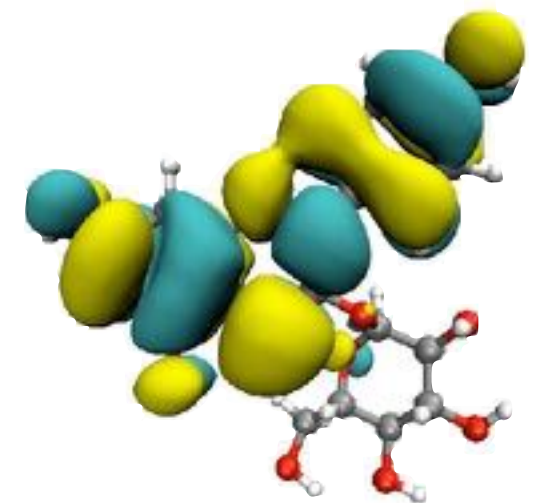
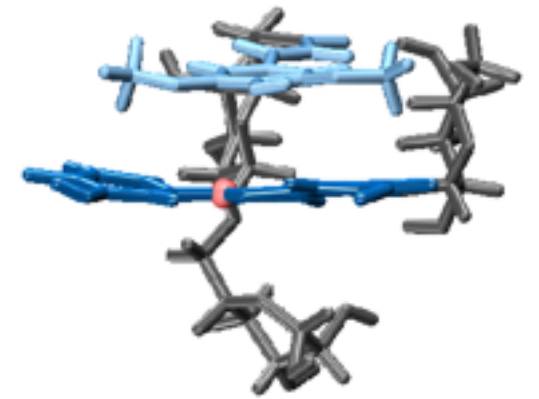
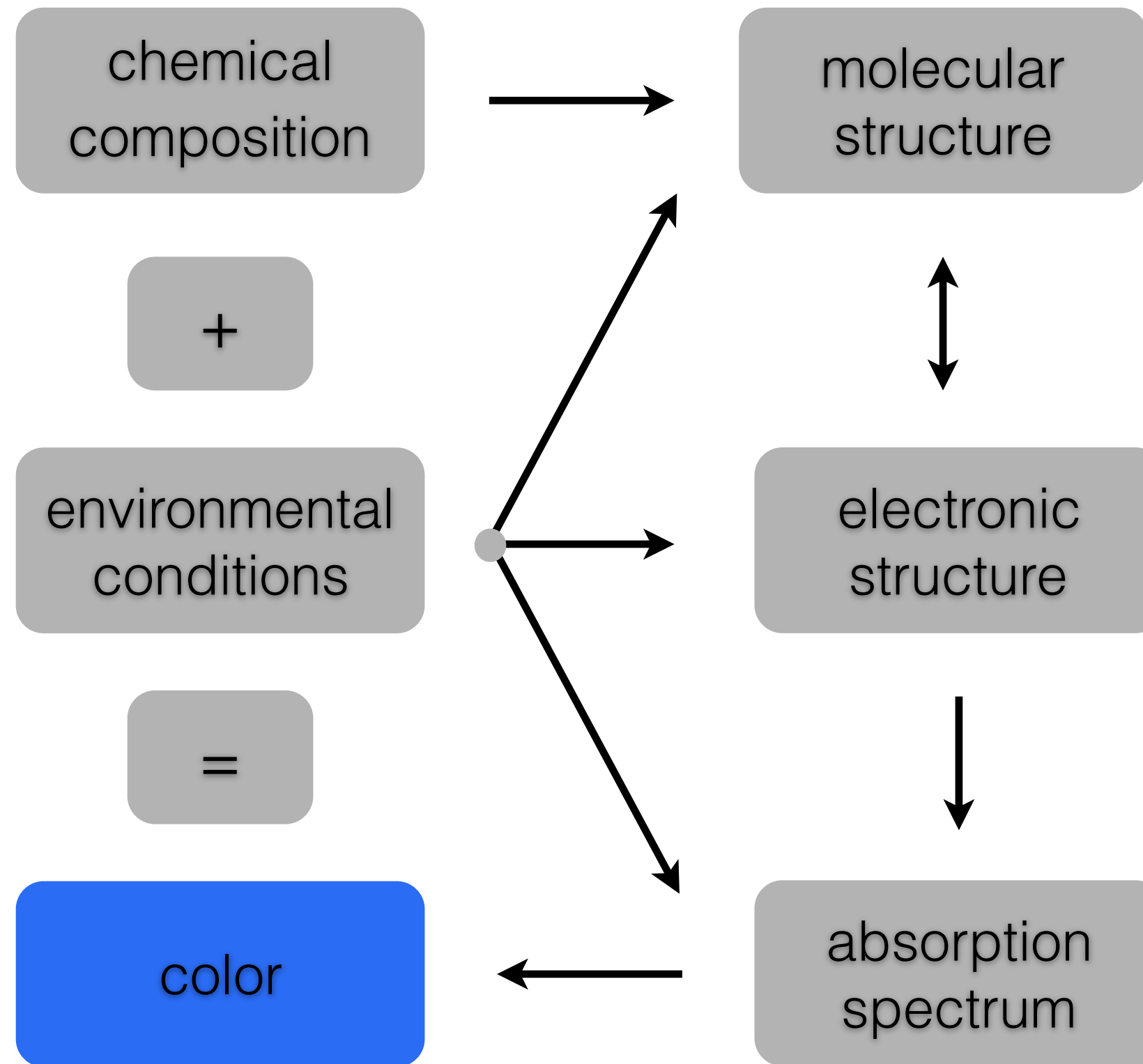
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the multiscale protocol

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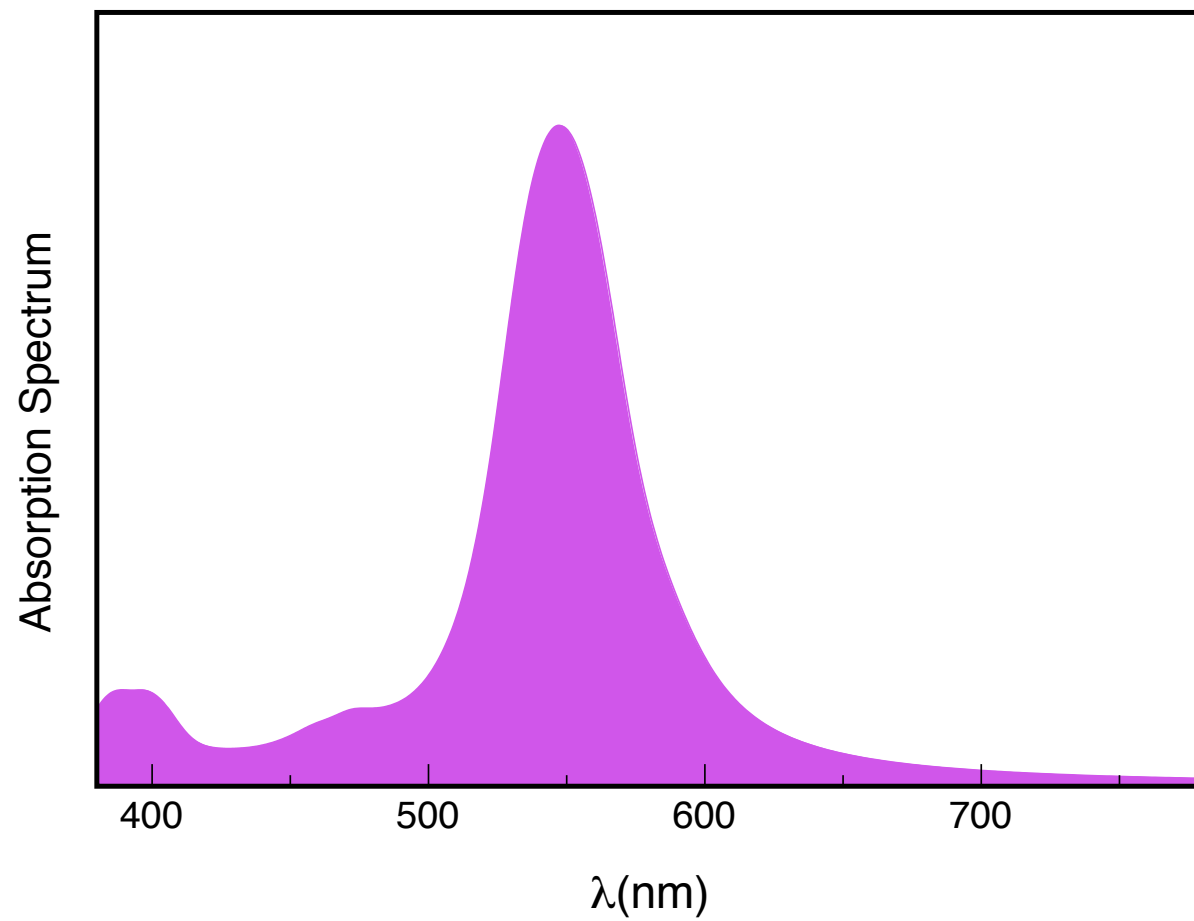
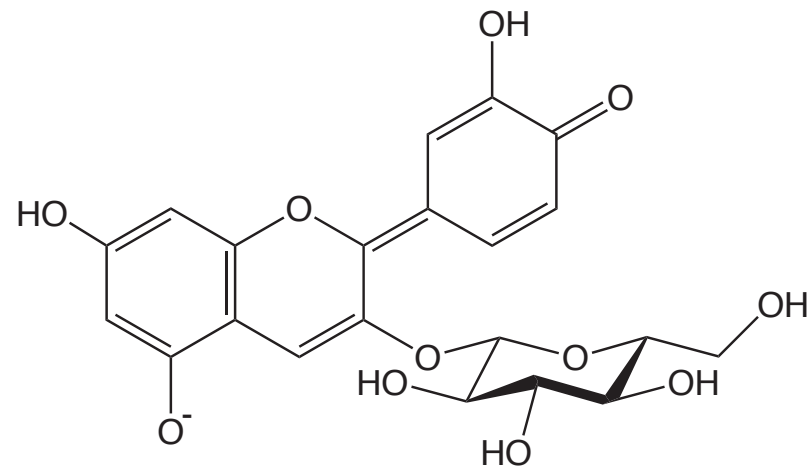
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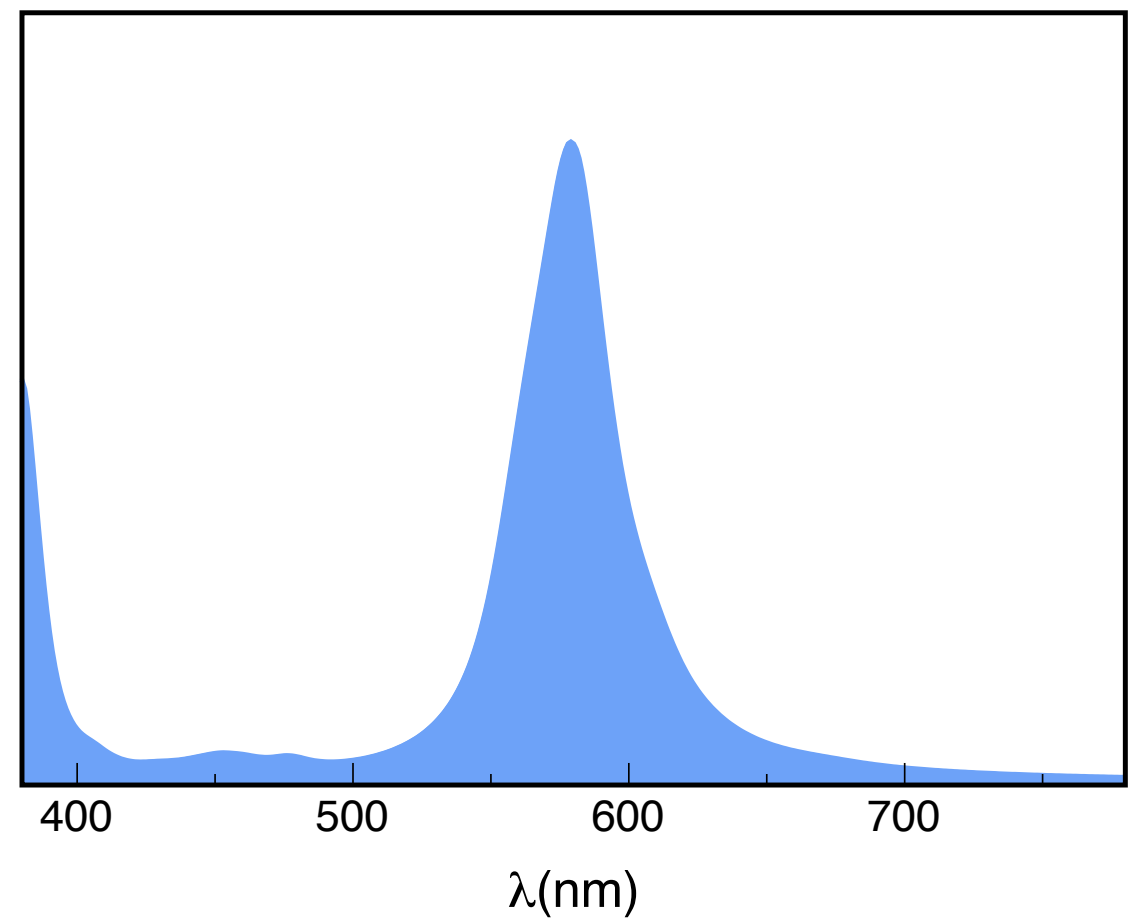
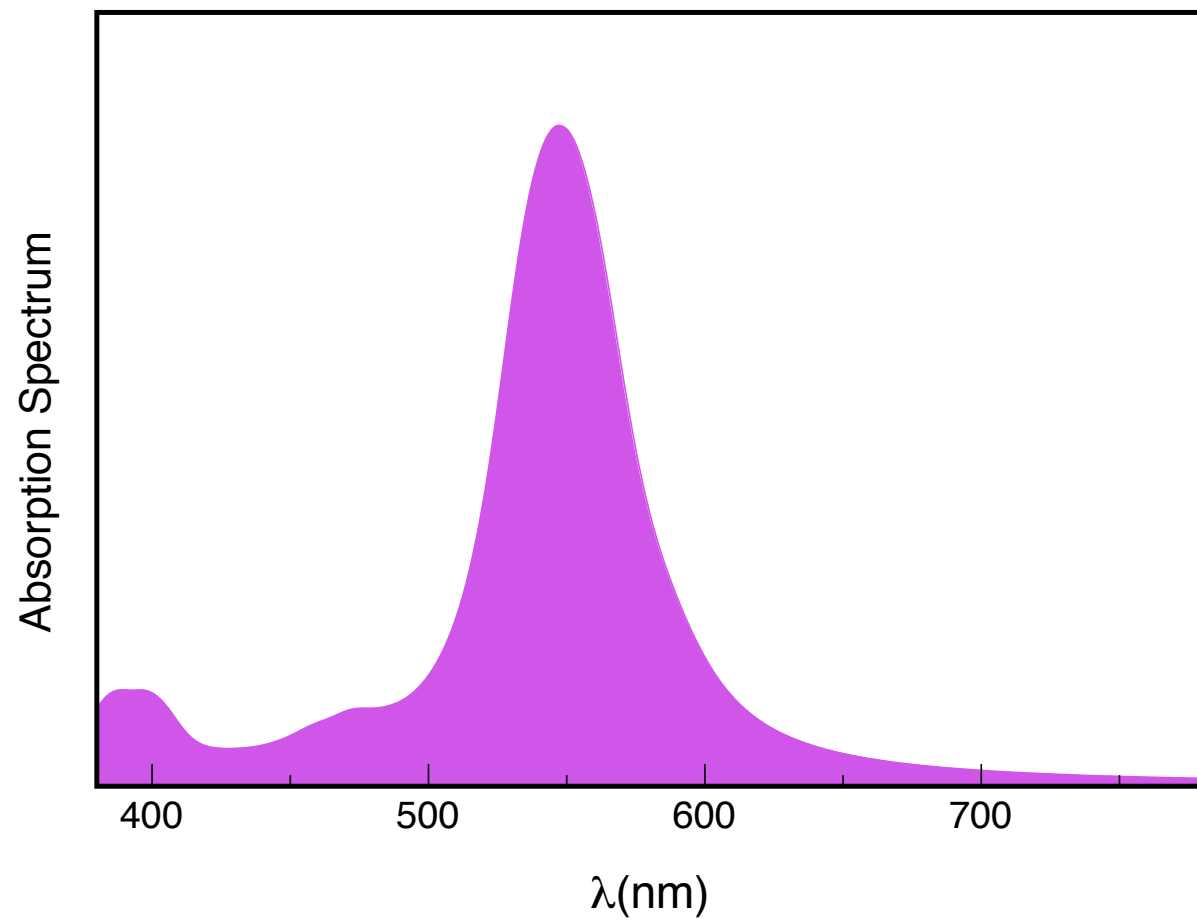
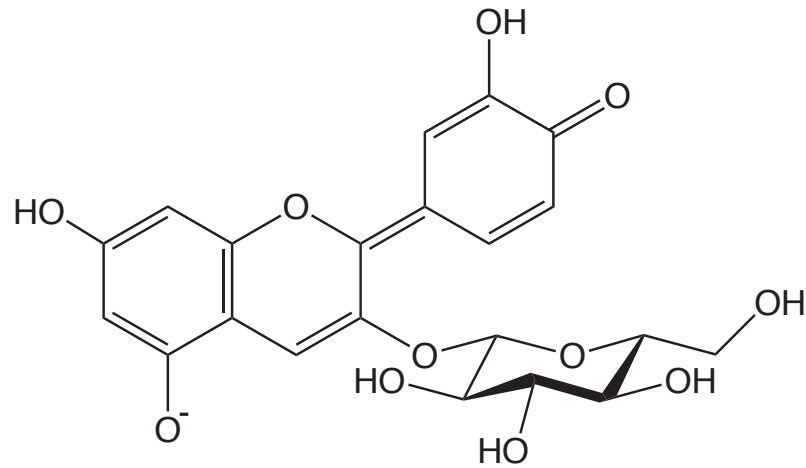
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6. **average** the spectra over different conformers, weighing with the populations computed in 1-2.



a newly identified substitute for “blue 2”



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



QUANTUMESPRESSO

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