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Substance concentrations

as conditions for the realization of dispositions

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Problem

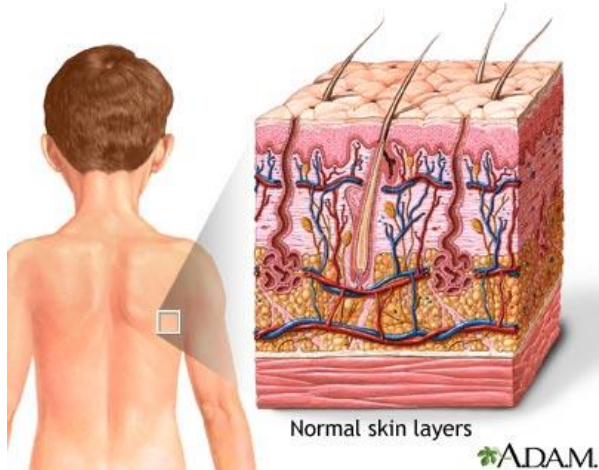Image credit: http://www.nlm.nih.gov/medlineplus

Ontologies make statements that are *universally true*

Image credit: http://www.topnews.in/health/files/Allergy.jpg

Dispositional properties specify what *might* occur under the right *circumstances*

Dispositions, functions

- Increasingly important in biomedical ontologies as they allow *functionally similar groupings* for entities that are *constitutionally dissimilar*, e.g. biologically active substances

- Realization: the process in which the disposition is 'fulfilled'

- Realization is *conditional*

Small molecule bioactivity

Drugs and metabolites: small molecules *active* in biological contexts
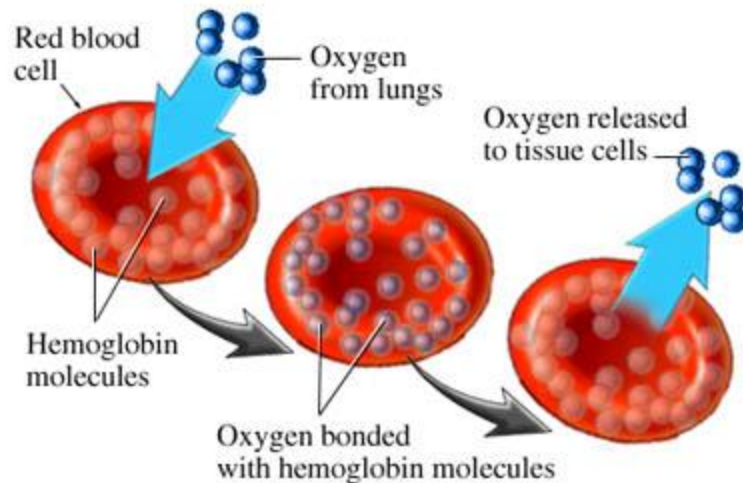

Red blood cell
Oxygen from lungs
Oxygen released to tissue cells
Hemoglobin molecules
Oxygen bonded with hemoglobin molecules

Image credit: gassama.myweb.uga.edu/

Oxygen transport in the body depends on

- the disposition of heme to **bind** oxygen
- and the disposition to **release** oxygen

binding affinity depends on the surrounding oxygen *concentration*

Concentrations

Concentrations are *system* properties
a concentration is always a concentration *of something in something*

e.g. the concentration of *alcohol* in *blood*
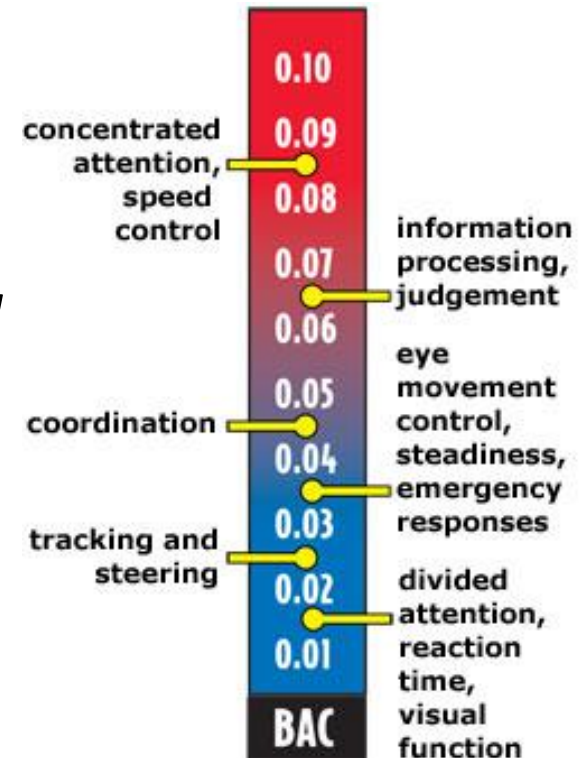
here shown in the Blood Alcohol Chart

Image credit: http://www.boat-ed.com/images/drawings/

Active concentrations

Consider aspirin as treatment for a headache

Image credit: tell.fll.purdue.edu

Too few individual molecules will have no effect
Too many tablets will have unpleasant additional effects

Conditions in biomedical ontologies

- Conditions for dispositional property realization, such as concentrations for active molecules, are seldom modelled explicitly in biomedical ontologies

- Such models are difficult to express in OWL binary relations

Ontology patterns for dispositions and concentration

Dispositions are realized
in *processes*
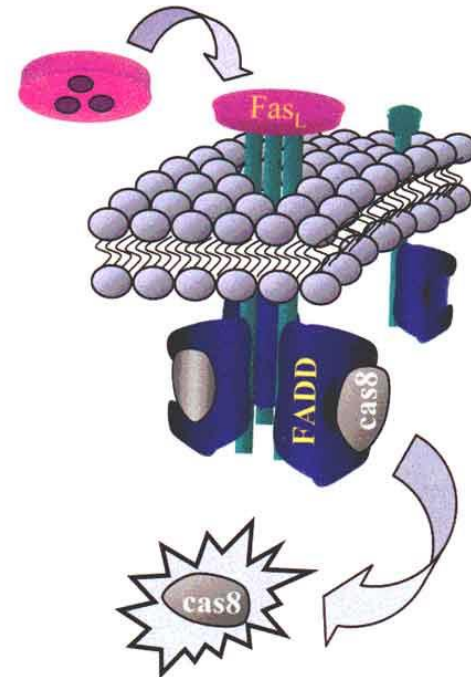
Model: Dispositions

Consider the case of aspirin, which has the disposition to treat pain.

We can formulate this as:

PortionOfAspirin ⊑ ∃ **bearerOf**.(*Disposition* ⊓

∀ **hasRealization**.(*Treating* ⊓ ∃ **hasParticipant**.*Pain*))

# Concentrations are properties of components of *mixtures*

Model: Concentrations

Consider a mixture of 10g water 🔴
with 10g glucose 🔴

(i)

We have three entities of interest

(i)   the water/glucose mixture wg_{mix}

(ii) the water fraction w_{coll} *i.e.*
      the collection of all water molecules

(ii)

(iii) the glucose fraction g_{coll} *i.e.*
      the collection of all glucose molecules.

(iii)

Bio-ontologies 2010: Substance concentrations as conditions for the realization
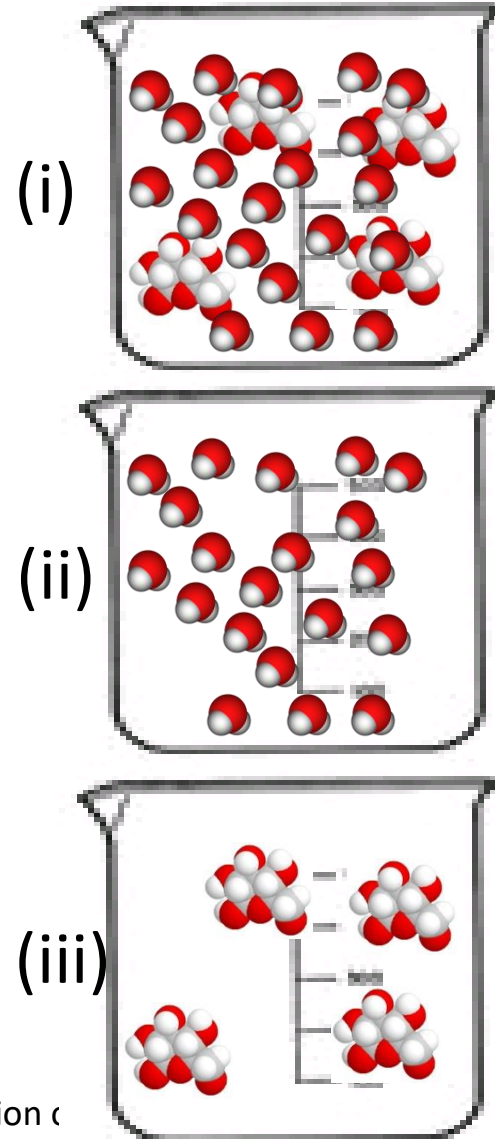
Model: Concentrations

Using BioTop relations **hasGranularPart** and **hasComponent**

The collection of glucose molecules in the water:

$$G \quad \sqsubseteq \quad EntireMolecule$$

$$G_{coll} \quad \sqsubseteq \quad HomogeneousCollection$$

$$G_{coll} \quad \equiv \quad \exists \textbf{ hasGranularPart}.G \sqcap \forall \textbf{ hasGranularPart}.G$$

A mixture has several components:

$$WG_{mix} \sqsubseteq \quad Mixture$$

$$WG_{mix} \sqsubseteq \quad =1 \textbf{ hasComponent}.G_{coll} \sqcap =1 \textbf{ hasComponent}.W_{coll}$$

Model: Concentrations

A concentration can be ascribed to a collection *iff* this collection is a component of a mixture

$\exists$ **bearerOf**.*Concentration* $\equiv$ *Homogeneous collection* $\sqcap$
$\exists$ **componentOf**.*Mixture*

Concentration $\sqsubseteq$ $\exists$ **inheresIn**. *(HomogeneousCollection* $\sqcap$
$\exists$ **componentOf**.*Mixture)*

Finally, we can state that

BloodGlucoseVolumeConcentration $\equiv$
VolumeConcentration $\sqcap$
$\exists$ **inheresIn**. *(PortionOfGlucose* $\sqcap$
$\exists$ **componentOf**.*PortionOfBlood)*

Dispositions and concentrations

The process, which realizes the disposition of a collection of molecules, can only occur when a *sufficient concentration* is available

Conditions for realization

How do we link the relevant conditions to the realization of dispositions? As a trigger (a circumstance without which a disposition cannot be realized):

$PortionOfAspirin \sqsubseteq \exists$ **bearerOf**.($Disposition \sqcap$
$\forall$ hasRealization.($Treating \sqcap \exists$ **hasParticipant**.$Pain \sqcap$
$\exists$ **hasTrigger**.$SufficientConcentration$))

where, of course,

$SufficientConcentration \sqsubseteq BloodAspirinVolumeConcentration.$

Conclusions

- Dispositional properties are fundamental to functional classification in Bio-ontologies

- Dispositional properties are defined in terms of their realization, but often realization also depends on *triggering conditions*

- One such triggering condition is the *concentration* of bioactive substances in the body

Acknowledgements