



Substance concentrations

as conditions for the realization of dispositions



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Problem

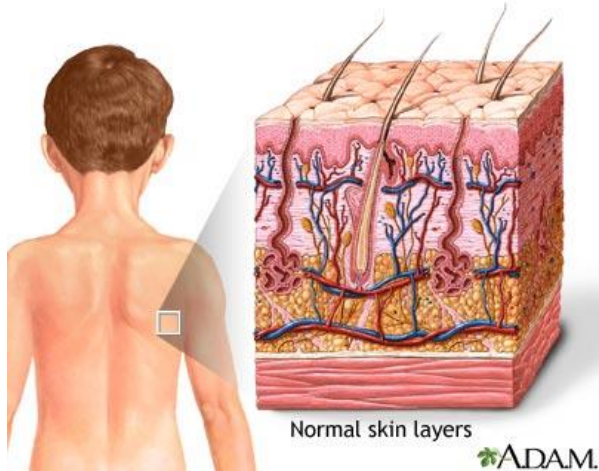


Image credit: <http://www.nlm.nih.gov/medlineplus>

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

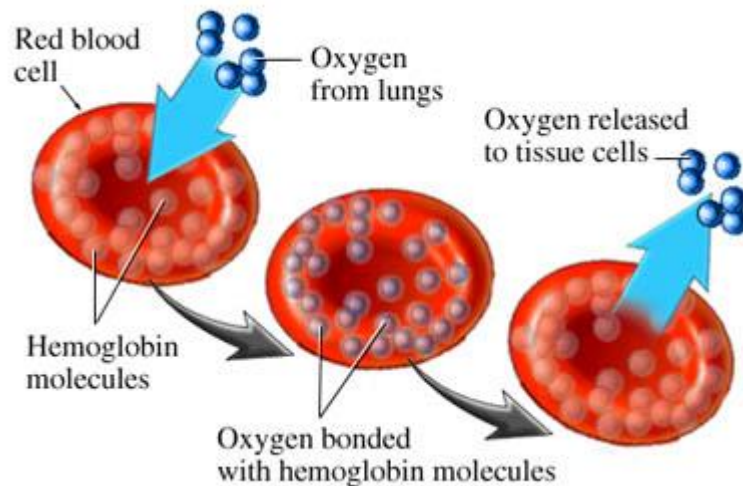


Image credit: gassama.myweb.uga.edu/

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

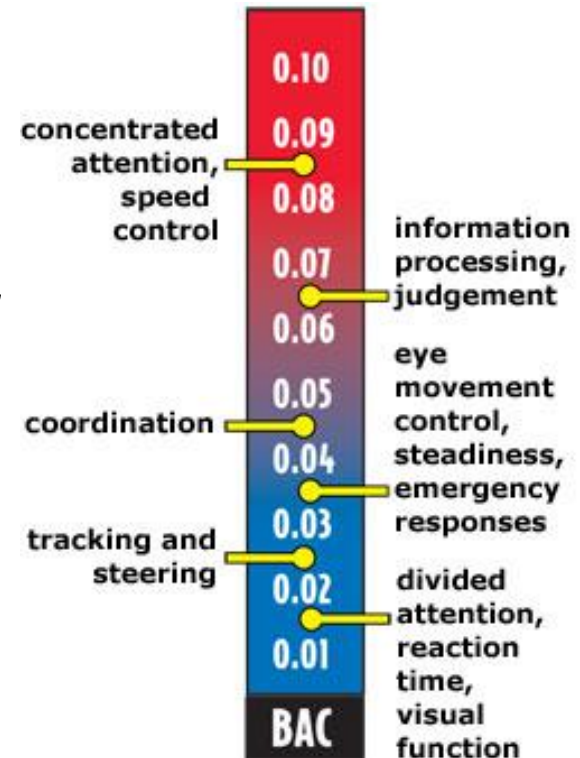


Image credit: <http://www.boat-ed.com/images/drawings/>

Active concentrations

Consider aspirin as treatment for a headache



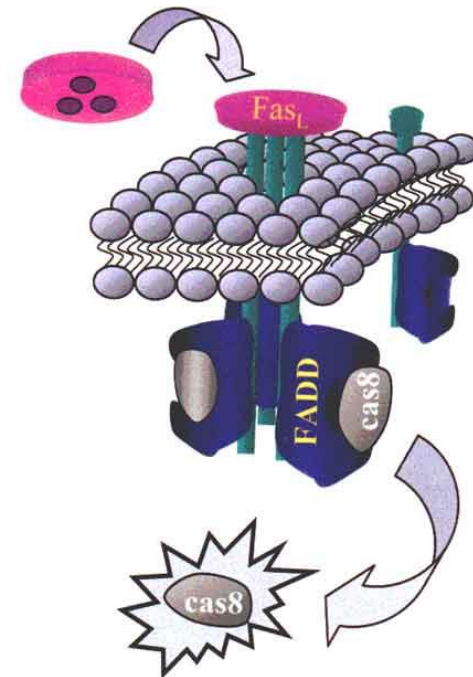
Too few individual molecules will have no effect
Too many tablets will have unpleasant additional effects

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:

$$\begin{aligned} \textit{PortionOfAspirin} \sqsubseteq \exists \textbf{bearerOf}.(\textit{Disposition} \sqcap \\ \forall \textbf{hasRealization}.(\textit{Treating} \sqcap \exists \textbf{hasParticipant}.\textit{Pain})) \end{aligned}$$

Concentrations are
properties of
components of
mixtures

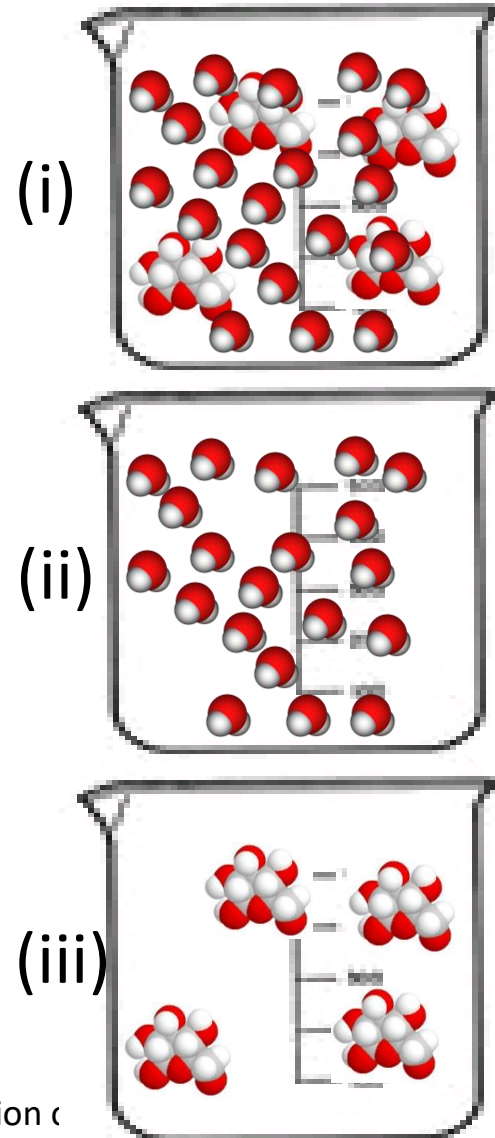


Model: Concentrations

Consider a mixture of 10g water  with 10g glucose 

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



Model: Concentrations

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

The collection of glucose molecules in the water:

$G \sqsubseteq \textit{EntireMolecule}$

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

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

A mixture has several components:

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

$WG_{mix} \sqsubseteq =1 \text{ hasComponent.G}_{coll} \sqcap =1 \text{ hasComponent.W}_{coll}$

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):

$$\textit{PortionOfAspirin} \sqsubseteq \exists \textbf{bearerOf} . (\textit{Disposition} \sqcap \forall \textit{hasRealization} . (\textit{Treating} \sqcap \exists \textbf{hasParticipant} . \textit{Pain} \sqcap \exists \textbf{hasTrigger} . \textit{SufficientConcentration}))$$

where, of course,

$$\textit{SufficientConcentration} \sqsubseteq \textit{BloodAspirinVolumeConcentration}.$$

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

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