

# WHODrug as Linked Data - an idea worth further exploration?

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## **WHO Collaborating Centre for International Drug Monitoring**



– Building a global safety culture

# Uppsala Monitoring Centre

Inspire. Engage. Transform.

Uppsala Monitoring Centre (UMC) advances the science of **pharmacovigilance** and inspires patient safety initiatives **all over the world**.

As an **independent, non-profit foundation**, we engage stakeholders who share our vision and collaborate to build a global patient safety culture.

As a leader in the research and **development of new scientific methods**, we explore the benefits and risks of medicines to help minimise harm to patients, and offer **products and services** used by health authorities and life-science companies worldwide.

For almost **40 years**, we have provided scientific leadership and operational support to the WHO Programme for International Drug Monitoring.



– Building a global safety culture

INSPIRE. ENGAGE. TRANSFORM.

# WHODrug™ Portfolio

Improving patient safety worldwide



– Building a global safety culture



- WHODrug Enhanced
- WHODrug China
- WHODrug Herbal
- WHODrug Japan CRT
- WHODrug Browser
- WHODrug ATC 5
- WHODrug SDGs
- WHODrug CAT



– Building a global safety culture

# WHODrug statistics

- **2 649 082 different medicinal products**, trade names with for example form and strength information added
- **369 789 unique names**

Product name ▼	Drug code	Active Ingredient(s)	ATC ⓘ	Country of sales	MAH	Pharmaceutical form	Strength
ARICLAIM	017493 02 004	Duloxetine hydrochloride	G04BX, Other urologicals <i>umc-assigned</i> • N02BG, Other analgesics and antipyretics <i>umc-assigned</i> • • N06AX, Other antidepressants <i>official</i>	Germany • Greece • Italy • Sweden	Boehringer ingelheim • Boehringer ingelheim italia • Eli Lilly and Company • Emra-med • Eurim-pharm • Gerke pharma • Lilly deutschland	CAPSULES • CAPSULES, ENTERIC-COATED • CAPSULES, OTHER	30 mg • 60 mg

# Deliv

Navigation icons: back, forward, and a search icon with the text "https".

Menu: File Edit View

Search: Google

Name

Requested R

Vigibase exp

WHODrug Cross Reference ATC5 Enhanced 2016 Sep 1

WHODrug Cross Reference ATC5 Enhanced and Herbal 2016 Sep 1

	ATC.txt	Text Document
	CCODE.txt	Text Document
	Format_C3-File_Descriptions.pdf	PDF File
	Format_C3-File_Diagram.pdf	PDF File
	ING.txt	Text Document
	MP.txt	Text Document
	ORG.txt	Text Document
	PF.txt	Text Document
	PP.txt	Text Document
	PRG.txt	Text Document
	PRT.txt	Text Document
	ReadMe.txt	Text Document
	SRCE.txt	Text Document
	STR.txt	Text Document
	SUN.txt	Text Document
	TableTotals.xls	Microsoft Excel 97-2003 Wor...
	THG.txt	Text Document
	UNIT.txt	Text Document
	Unit-L.txt	Text Document
	Unit-X.txt	Text Document
	Version.txt	Text Document

Navigation icons: close, maximize, and a search icon with the text "https".

Menu: File Edit View

Search: Google

Name

Requested R

Vigibase exp

WHODrug Cross Reference ATC5 Enhanced 2016 Sep 1

WHODrug Cross Reference ATC5 Enhanced and Herbal 2016 Sep 1



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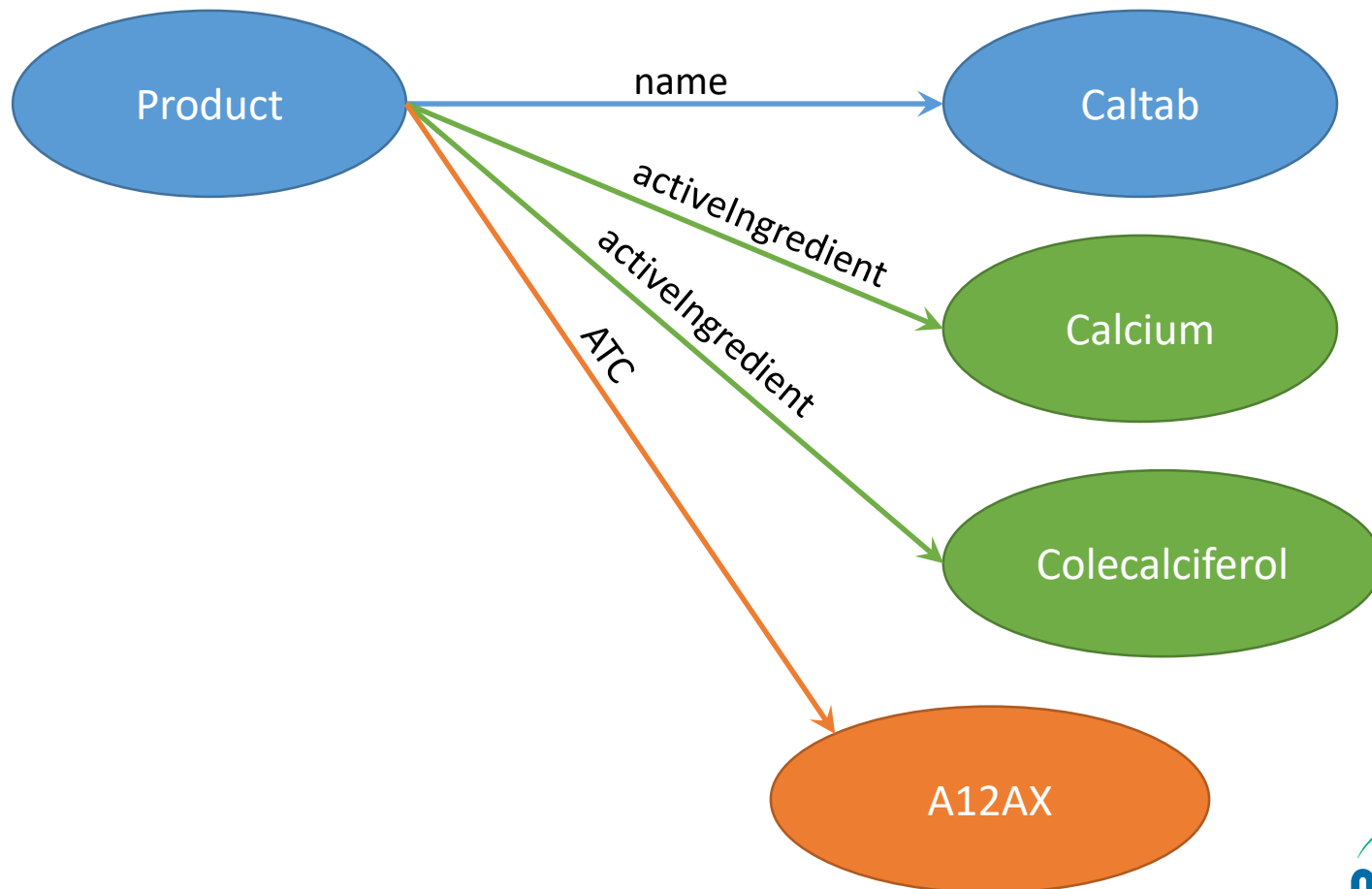
- WHODrug Enhanced
- WHODrug China
- WHODrug Herbal
- WHODrug Japan CRT
- WHODrug Browser
- WHODrug ATC 5
- WHODrug SDGs
- WHODrug CAT



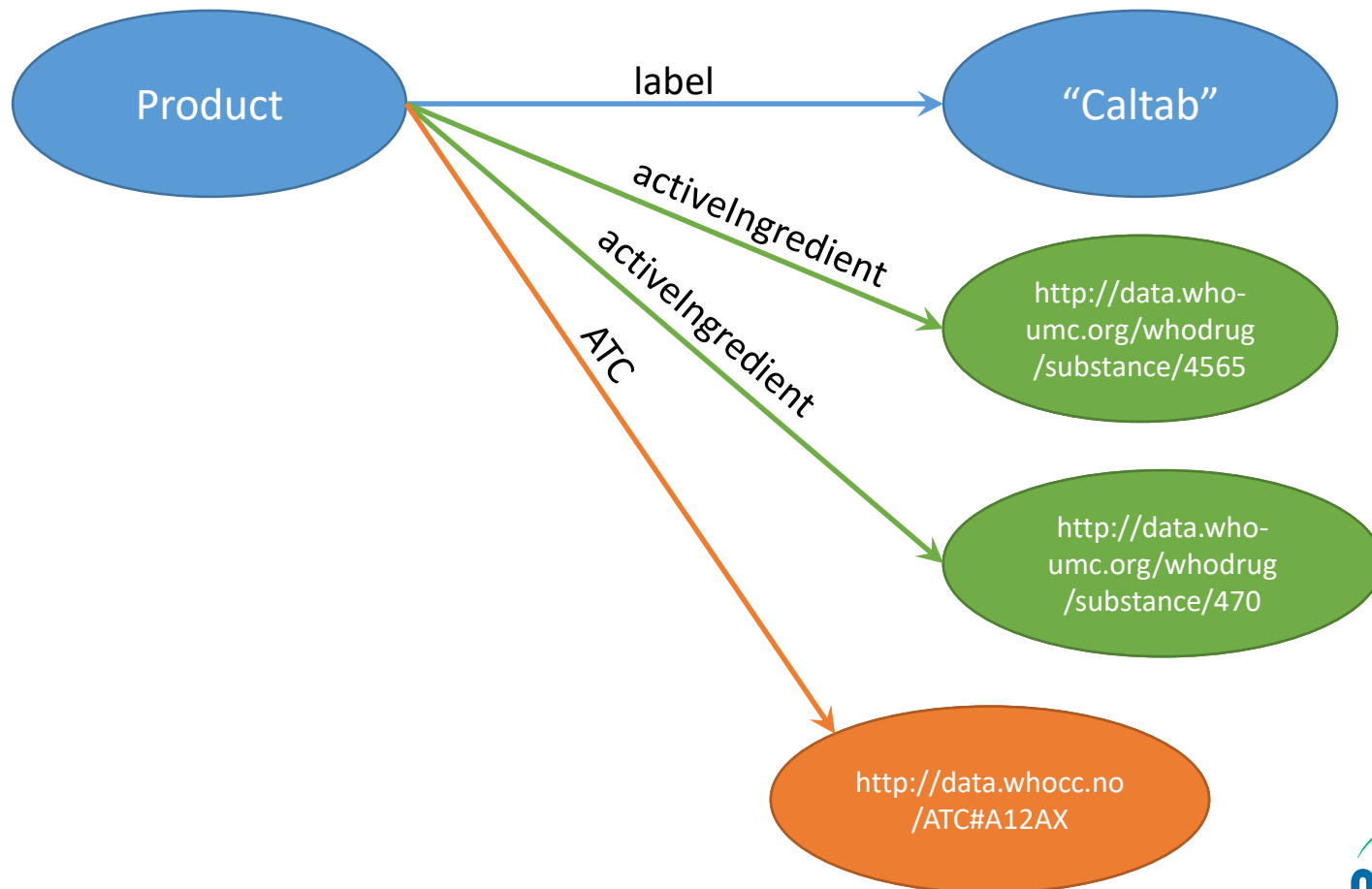
– Building a global safety culture



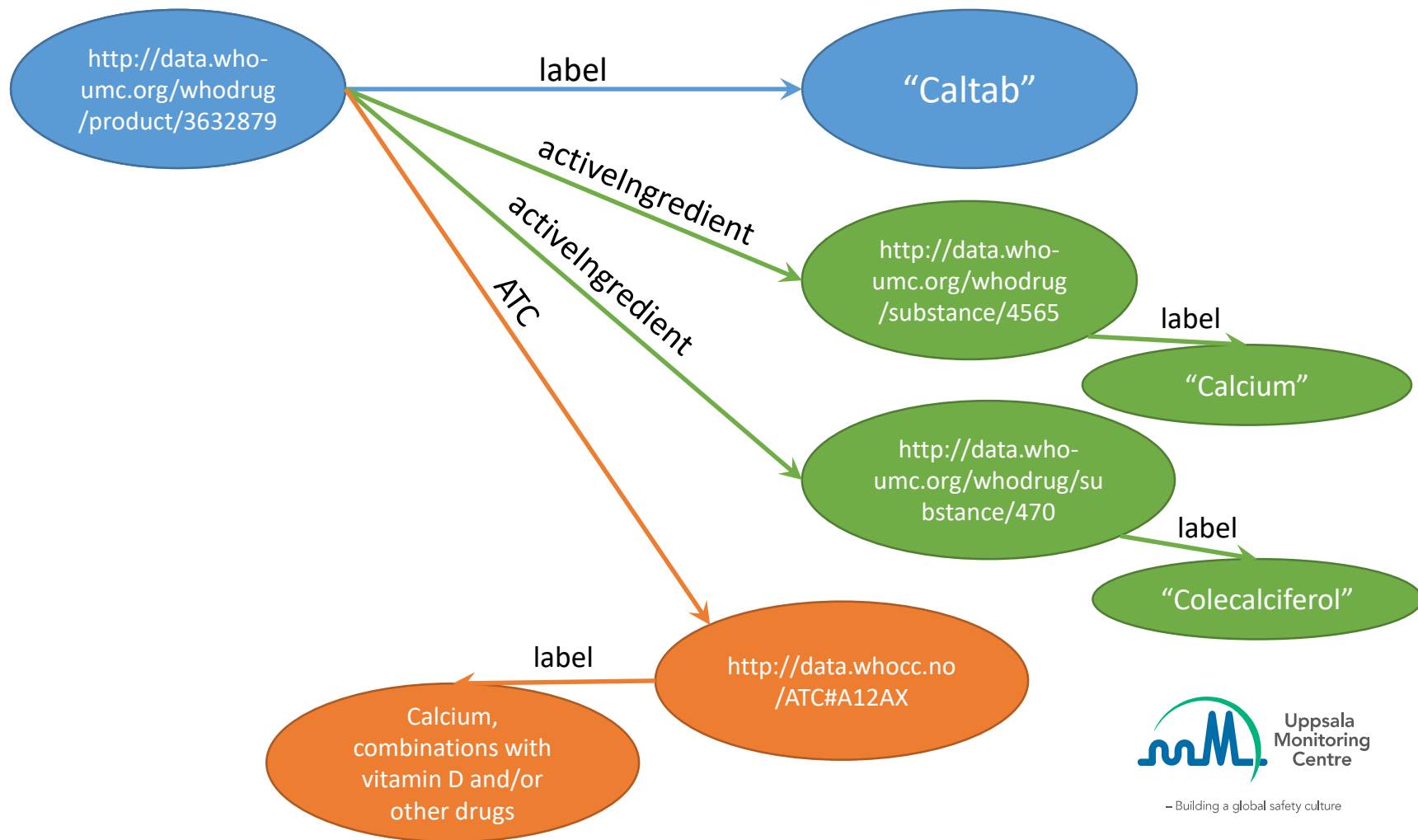
# Why Linked Data



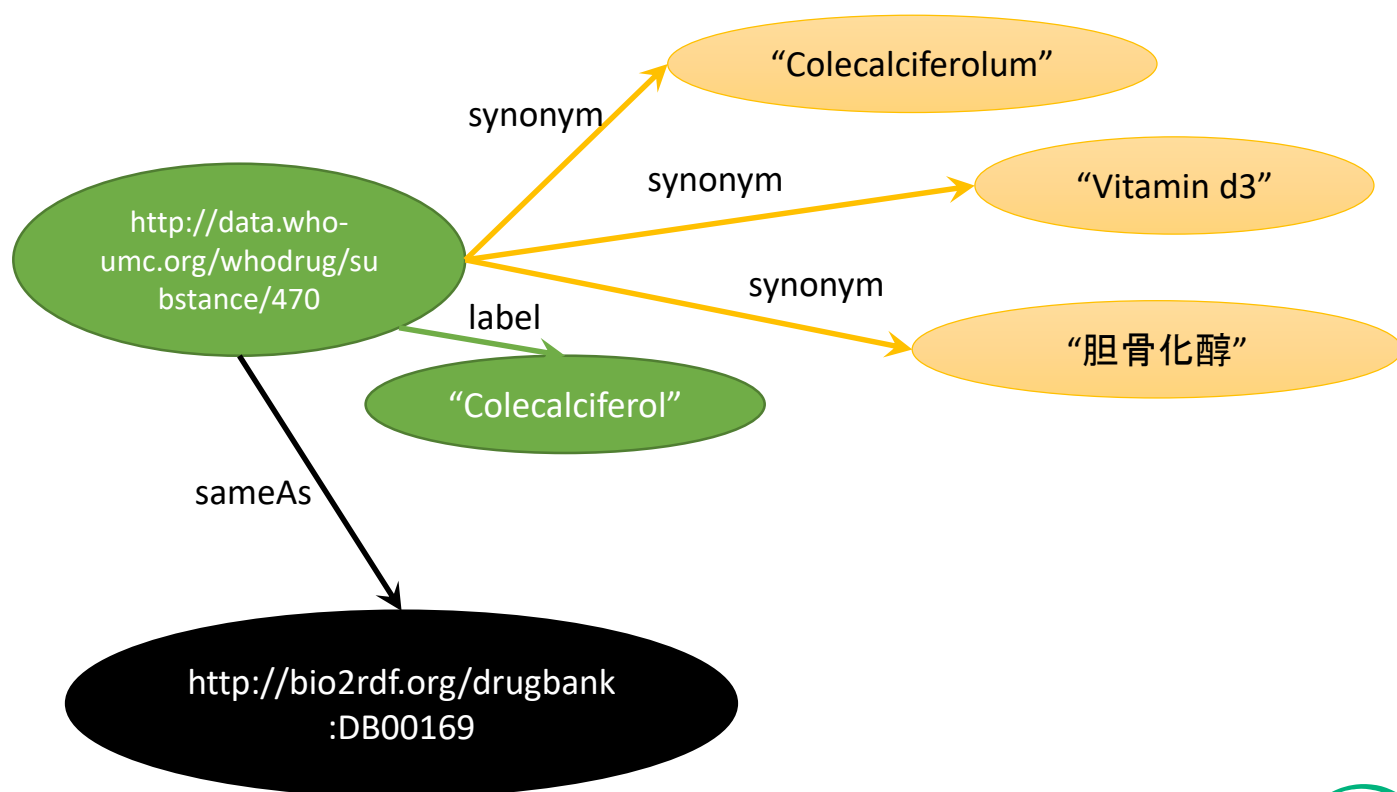
# Why Linked Data



# Why Linked Data



# Why Linked Data - Exploring a substance



# Key benefit of using a URI as identifier

Caltab

Calcium Carbonate

<http://data.who-umc.org/whodrug/product/2359181>

Caltab

Calcium, Colecalciferol

<http://data.who-umc.org/whodrug/product/3750822>

# Usage of the URIs

```
- <drug>
  <drugcharacterization>1</drugcharacterization>
  <medicinalproduct>http://data.who-umc.org/whodrug/product/3750822
  <druginterval dosageunitnumb/>
  <druginterval dosagedefinition/>
  <drugdosagetext>2 tablets daily</drugdosagetext>
  <drugadministrationroute/>
  <drugindicationmeddraversion>19.0</drugindicationmeddraversion>
  <drugindication/>
  <actiondrug/>
  <drugadditional>Strength: Reason for taking drug: </drugadditional>
- <activesubstance>
  <activesubstancename/>
  </activesubstance>
  <drugreactionrelatedness/>
</drug>
```

# General identification of medicinal products

The patient took Caltab as a concomitant medication during the trial...



# Resolving the URI (in a web-browser)



## Details about: Caltab

Record Type	TradeNameRecordLevel1
Name Specifier	
Drug Code	13500101098
Old Form	False
Medicinal Product ID	3750822
Active ingredients	Calcium Colecalciferol
ATC classification	A12AX Calcium, combinations with vitamin D and/or other drugs
Create date	20161205
Narrower	<a href="http://localhost/Umc.VigiFlowLookup/medicinalproduct/3750822/narrower">http://localhost/Umc.VigiFlowLookup/medicinalproduct/3750822/narrower</a>



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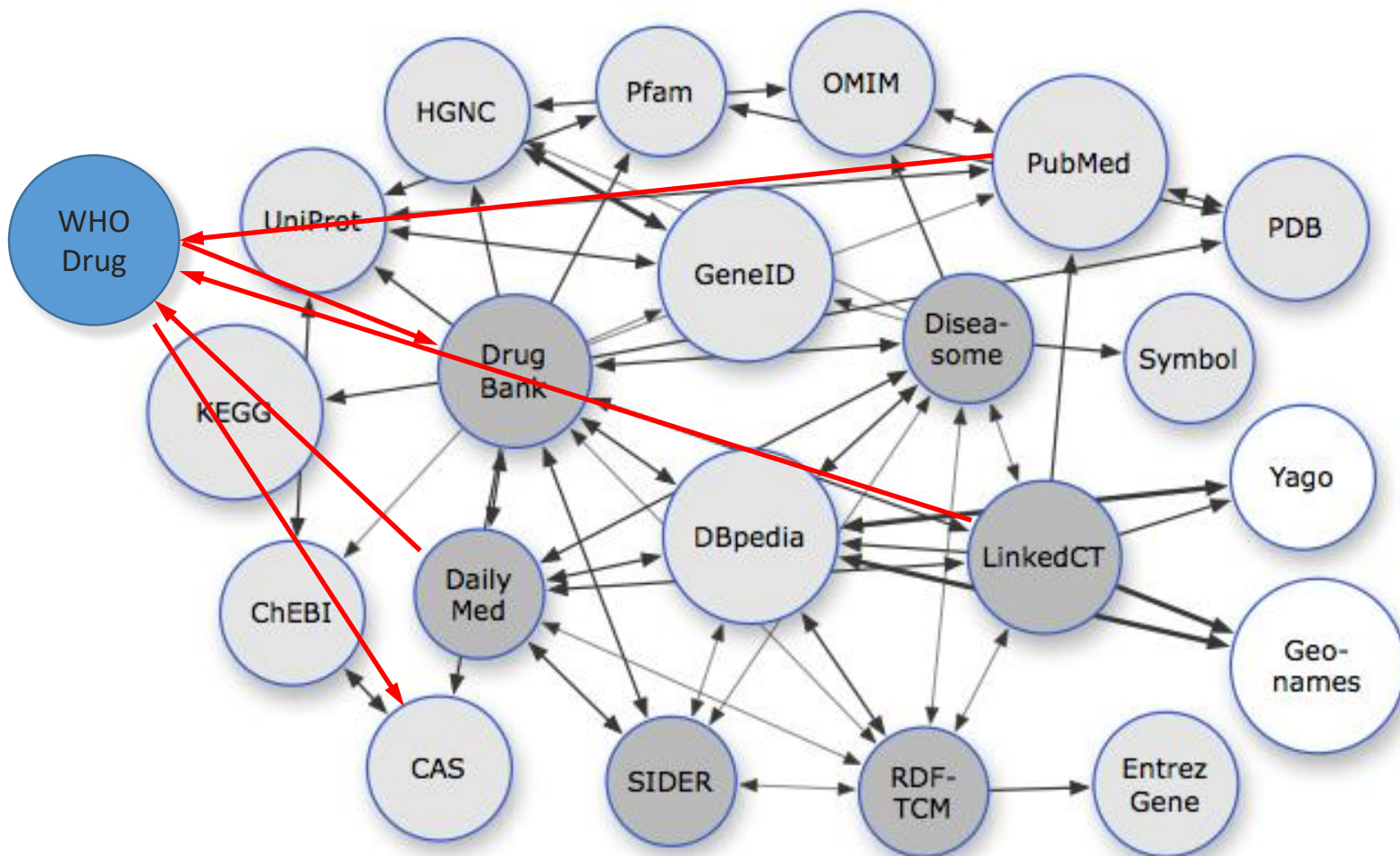
© Uppsala Monitoring Centre



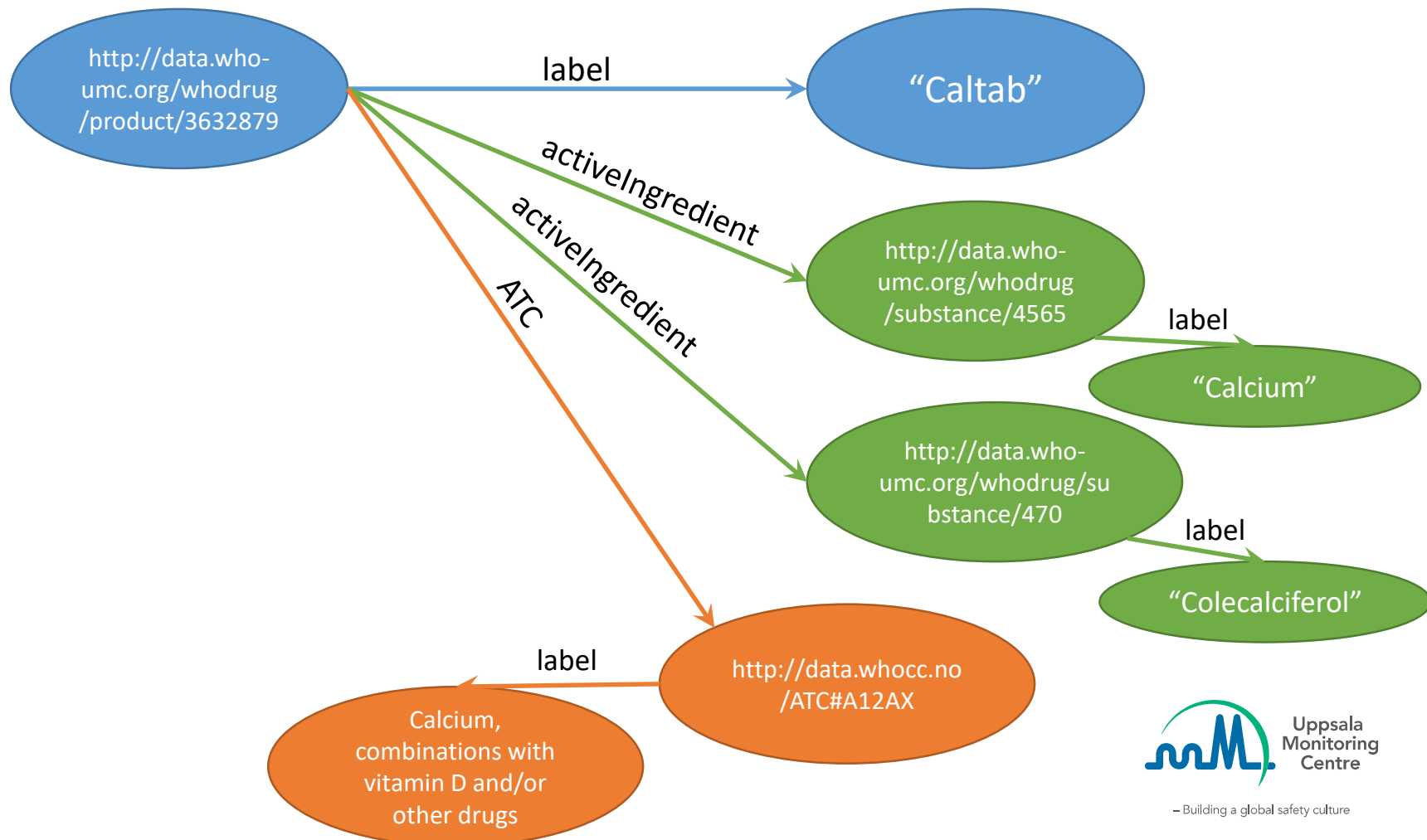
# Resolving the URI from a system (Accept: application/xml or json)

```
<TradeNameRecordLevel1>
  <@context> "http://data.who-umc.org:8080/whodrug/schema/Product.jsonld",
  <@id> "http://localhost/Umc.VigiFlowLookup/data/product/3750822",
  <@type> "TradeNameRecordLevel1",
  <productId> 3750822,
  <name> "Caltab",
  <nameSpecifier> "",
  <drugCode> "13500101098",
  <createDate> "20161205",
  <narrower> "http://localhost/Umc.VigiFlowLookup/data/product/3750822/narrower",
  <activeIngredients> [
    {
      <substance> "http://localhost/Umc.VigiFlowLookup/data/substance/4565",
      <substanceId> 4565,
      <substanceName> "Calcium",
      <strength> null
    },
    {
      <substance> "http://localhost/Umc.VigiFlowLookup/data/substance/470",
      <substanceId> 470,
```

# WHODrug as linked data



# From conceptual model to Linked Data

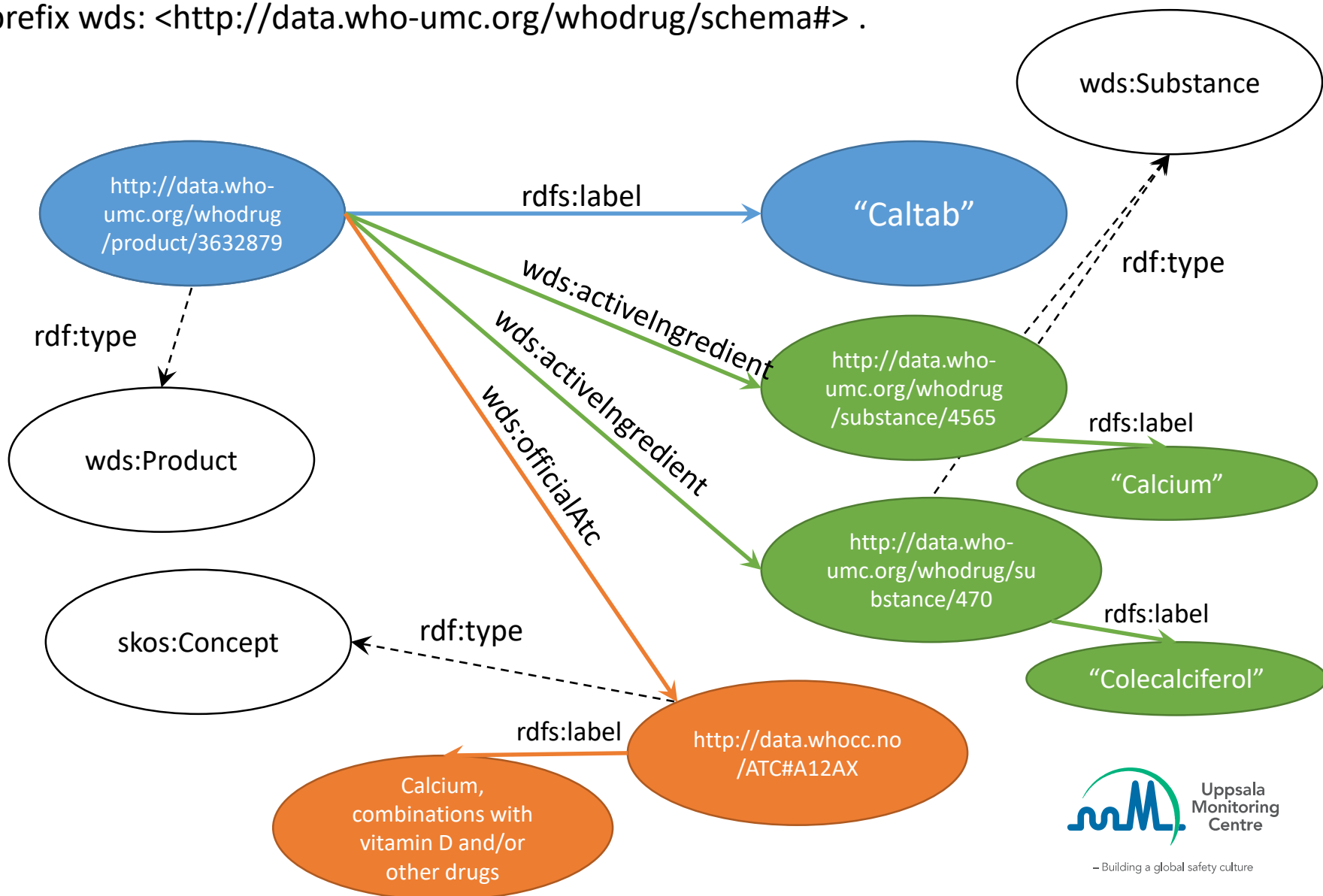


@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .



















@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .

@prefix skos: <http://www.w3.org/2004/02/skos/core#> .

@prefix wds: <http://data.who-umc.org/whodrug/schema#> .



# The conceptual model as a linked data schema (RDF)

 <a href="http://data.who-umc.org/whodrug/schema#SubstanceCode">http://data.who-umc.org/whodrug/schema#SubstanceCode</a>	 <a href="#">rdf:type</a>	 <a href="#">owl:Class</a>
 <a href="http://data.who-umc.org/whodrug/schema#SubstanceCode">http://data.who-umc.org/whodrug/schema#SubstanceCode</a>	 <a href="#">skos:definition</a>	A Substance Code is an identifier for a substance which some meaning built into it, such as a reference to another source.
 <a href="http://data.who-umc.org/whodrug/schema#CasNumber">http://data.who-umc.org/whodrug/schema#CasNumber</a>	 <a href="#">skos:definition</a>	A CAS Number is a CAS Registry Number assigned by Chemical Abstracts Service.
 <a href="http://data.who-umc.org/whodrug/schema#CasNumber">http://data.who-umc.org/whodrug/schema#CasNumber</a>	 <a href="#">rdfs:subClassOf</a>	 <a href="http://data.who-umc.org/whodrug/schema#SubstanceCode">http://data.who-umc.org/whodrug/schema#SubstanceCode</a>
 <a href="http://data.who-umc.org/whodrug/schema#HerbalCode">http://data.who-umc.org/whodrug/schema#HerbalCode</a>	 <a href="#">skos:definition</a>	A Herbal Code Number is a sequence divided into three parts which makes it possible to identify the plant, the part of the plant and the extraction method for herbal substances. This in turn makes it possible to analyze more data with respect to these parameters.
 <a href="http://data.who-umc.org/whodrug/schema#HerbalCode">http://data.who-umc.org/whodrug/schema#HerbalCode</a>	 <a href="#">rdfs:subClassOf</a>	 <a href="http://data.who-umc.org/whodrug/schema#SubstanceCode">http://data.who-umc.org/whodrug/schema#SubstanceCode</a>
 <a href="http://data.who-umc.org/whodrug/schema#Substance">http://data.who-umc.org/whodrug/schema#Substance</a>	 <a href="#">rdf:type</a>	 <a href="#">owl:Class</a>

# SPARQL Query

```
PREFIX wds: <http://data.who-umc.org/whodrug/schema#>

select ?product ?tradenname ?country ?substances from <http://data.who-umc.org/whodrug>
where {?product rdf:type wds:TradeNameRecord .
      ?product rdfs:label ?tradenname .
      FILTER regex(?tradenname, "^Calta", "i")
      ?product wds:marketingCountry ?country .
      ?product wds:productComposition ?comp .
      ?comp rdfs:label ?substances
} limit 10
```



















## SPARQL Results

product	tradenname	country	substances
<a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	Caltab	<a href="http://data.who-umc.org/whodrug/concept/country#356">http://data.who-umc.org/whodrug/concept/country#356</a>	Calcium;Colecalciferol
<a href="http://data.who-umc.org/whodrug/product/073570.01.302">http://data.who-umc.org/whodrug/product/073570.01.302</a>	Caltab	<a href="http://data.who-umc.org/whodrug/concept/country#586">http://data.who-umc.org/whodrug/concept/country#586</a>	Calcium carbonate
<a href="http://data.who-umc.org/whodrug/product/073570.01.302">http://data.who-umc.org/whodrug/product/073570.01.302</a>	Caltab	<a href="http://data.who-umc.org/whodrug/concept/country#764">http://data.who-umc.org/whodrug/concept/country#764</a>	Calcium carbonate
<a href="http://data.who-umc.org/whodrug/product/073570.01.383">http://data.who-umc.org/whodrug/product/073570.01.383</a>	Caltan	<a href="http://data.who-umc.org/whodrug/concept/country#392">http://data.who-umc.org/whodrug/concept/country#392</a>	Calcium carbonate



# Describe the product

<http://data.who-umc.org/whodrug/product/3632879>

 <a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	 <a href="#">rdf:type</a>	 <a href="http://data.who-umc.org/whodrug/schema#TradeNameRe">http://data.who-umc.org/whodrug/schema#TradeNameRe</a>
 <a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	 <a href="http://data.who-umc.org/whodrug/schema#productComposition">http://data.who-umc.org/whodrug/schema#productComposition</a>	 <a href="http://data.who-umc.org/whodrug/composition/13500101">http://data.who-umc.org/whodrug/composition/13500101</a>
 <a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	 <a href="http://data.who-umc.org/whodrug/schema#sequence2">http://data.who-umc.org/whodrug/schema#sequence2</a>	098
 <a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	 <a href="http://data.who-umc.org/whodrug/schema#marketingCountry">http://data.who-umc.org/whodrug/schema#marketingCountry</a>	 <a href="http://data.who-umc.org/whodrug/concept/country#356">http://data.who-umc.org/whodrug/concept/country#356</a>
 <a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	 <a href="http://data.who-umc.org/whodrug/schema#officialAtc">http://data.who-umc.org/whodrug/schema#officialAtc</a>	 <a href="http://data.whocc.no/ATC#A12AX">http://data.whocc.no/ATC#A12AX</a>
 <a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	 <a href="#">rdfs:label</a>	Caltab
 <a href="http://data.who-umc.org/whodrug/product/135001.01.098">http://data.who-umc.org/whodrug/product/135001.01.098</a>	 <a href="http://data.who-umc.org/whodrug/schema#createDate">http://data.who-umc.org/whodrug/schema#createDate</a>	2016-12-05



















# Describe the product composition

<http://data.who-umc.org/whodrug/composition/13500101>

<a href="http://data.who-umc.org/whodrug/composition/13500101">http://data.who-umc.org/whodrug/composition/13500101</a>	<a href="#">rdf:type</a>	<a href="http://data.who-umc.org/whodrug/schema#BaseComposition">http://data.who-umc.org/whodrug/schema#BaseComposition</a>
<a href="http://data.who-umc.org/whodrug/composition/13500101">http://data.who-umc.org/whodrug/composition/13500101</a>	<a href="http://data.who-umc.org/whodrug/schema#drugCode">http://data.who-umc.org/whodrug/schema#drugCode</a>	<a href="http://data.who-umc.org/whodrug/composition/135001">http://data.who-umc.org/whodrug/composition/135001</a>
<a href="http://data.who-umc.org/whodrug/composition/13500101">http://data.who-umc.org/whodrug/composition/13500101</a>	<a href="http://data.who-umc.org/whodrug/schema#activeIngredient">http://data.who-umc.org/whodrug/schema#activeIngredient</a>	<a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>
<a href="http://data.who-umc.org/whodrug/composition/13500101">http://data.who-umc.org/whodrug/composition/13500101</a>	<a href="http://data.who-umc.org/whodrug/schema#activeIngredient">http://data.who-umc.org/whodrug/schema#activeIngredient</a>	<a href="http://data.who-umc.org/whodrug/substance/4565">http://data.who-umc.org/whodrug/substance/4565</a>
<a href="http://data.who-umc.org/whodrug/composition/13500101">http://data.who-umc.org/whodrug/composition/13500101</a>	<a href="http://data.who-umc.org/whodrug/schema#sequence1">http://data.who-umc.org/whodrug/schema#sequence1</a>	01
<a href="http://data.who-umc.org/whodrug/composition/13500101">http://data.who-umc.org/whodrug/composition/13500101</a>	<a href="#">rdfs:label</a>	Calcium;Colecalciferol

# Describe the substance

<http://data.who-umc.org/whodrug/substance/470>

 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 <a href="http://data.who-umc.org/whodrug/schema#synonym">http://data.who-umc.org/whodrug/schema#synonym</a>	Cholecalciferol
 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 <a href="http://data.who-umc.org/whodrug/schema#synonym">http://data.who-umc.org/whodrug/schema#synonym</a>	Cholecalciferolum
 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 <a href="http://data.who-umc.org/whodrug/schema#synonym">http://data.who-umc.org/whodrug/schema#synonym</a>	Vitamina d3
 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 <a href="http://data.who-umc.org/whodrug/schema#synonym">http://data.who-umc.org/whodrug/schema#synonym</a>	Kolecalciferol
 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 <a href="http://data.who-umc.org/whodrug/schema#synonym">http://data.who-umc.org/whodrug/schema#synonym</a>	Colecalciferolum
 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 <a href="http://data.who-umc.org/whodrug/schema#synonym">http://data.who-umc.org/whodrug/schema#synonym</a>	胆骨化醇
 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 <a href="http://data.who-umc.org/whodrug/schema#substanceCode">http://data.who-umc.org/whodrug/schema#substanceCode</a>	 <a href="http://data.who-umc.org/whodrug/substance/0000067970">http://data.who-umc.org/whodrug/substance/0000067970</a>
 <a href="http://data.who-umc.org/whodrug/substance/470">http://data.who-umc.org/whodrug/substance/470</a>	 owl:sameAs	 <a href="http://bio2rdf.org/drugbank:DB00169">http://bio2rdf.org/drugbank:DB00169</a>

# Moving forward

**Do nothing**

**Deliver a schema – leave implementation to users (based on old text files)**

**Deliver schema and data as RDF-files (version controlled)**

**Deliver a Linked Data API with resolvable URIs (HTML, json-LD, RDF)**

**SPARQL-endpoint**

# WHODrug as Linked Data - an idea worth further exploration?



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