



Bethesda, Maryland  
May 11, 2006

# Biomedical Ontology And Drug Information



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# Outline

- ◆ Drug vocabularies
- ◆ Drug vocabulary integration: **UMLS**
- ◆ Drug vocabulary standardization: **RxNorm**
- ◆ Visualization and processing of drug information: **RxNav**



# Drug Vocabularies

# Drug vocabularies

- ◆ Master Drug Data Base  
(Medi-Span, Wolters Kluwer Health)
- ◆ Multum MediSource Lexicon
- ◆ Micromedex DRUGDEX
- ◆ FDA National Drug Code Directory
- ◆ Nat'l Drug Data File Plus Source Vocabulary  
(First DataBank Inc.)
- ◆ Veterans Health Administration National Drug  
File





# Drugs in SNOMED CT

Apelon Mycroft - SNOMED CT (July 2005)

File Favorites Help

Tree Walker Search

- SNOMED CT Concept (SNOMED RT+CTV3)
  - Body structure (body structure)
  - Clinical finding (finding)
  - Context-dependent categories (context-dependent category)
  - Environments and geographical locations (environment / location)
  - Events (event)
  - Linkage concept (linkage concept)
  - Observable entity (observable entity)
  - Organism (organism)
  - Pharmaceutical / biologic product (product)**
  - Physical force (physical force)
  - Physical object (physical object)
  - Procedure (procedure)
  - Qualifier value (qualifier value)
  - Social context (social concept)
  - Special concept (special concept)
  - Specimen (specimen)
  - Staging and scales (staging scale)
  - Substance (substance)

Concept

Pharmaceutical / biologic product (product)

- Pharmaceutical / biologic product (product)
  - Namespace: SNOMED CT
  - Synonyms
    - Drug
    - Drug product
    - Medicinal product
    - Pharmaceutical / biologic product ( Preferred )
    - Pharmaceutical / biologic product (product)
  - Properties
    - Code in Source: 373873005
    - Concept Status: Current
    - NHS Clinical Terms Version 3: XUWOO
    - SNOMED Legacy-style Code: R-003EB
    - subset: H
    - UMLS CUI: C0013227
    - UMLS Semantic Type: Pharmacologic Substance
  - Roles
  - Associations





# Drugs in SNOMED CT

- Pharmaceutical / biologic product (product)
- Alternative medicines (product)
- Analgesic (product)
- Anesthetic (product)
- Antiallergenic drugs (product)
- Antidiabetic preparation (product)
- Anti-infective agent (product)
- Antineoplastic agent (product)
- Autonomic drug (product)
- Biological agent (product)
- Blood product (product)
- Bone resorption inhibitor (product)
- Cardiovascular drug (product)
- Chelating agents and antidotes (product)
- CNS drug (product)
- Collagen product (product)
- Diagnostic aid (product)
- Dietary product (product)
- Drug groups primarily affecting the musculoskeletal system (product)
- Drug values (product)
- Drug-device combination product (product)
- Drugs used in metabolic disorders (product)
- Drugs used in the eye (product)
- Enzyme inhibitor (product)

- Enzyme inhibitor (product)
- Enzyme preparation (product)
- Gastrointestinal drug (product)
- Gelatin (product)
- Genital system agent (product)
- Hematologic drug (product)
- Hormone preparation (product)
- Immunotherapeutic agent (product)
- Miscellaneous products (product)
- Nasal preparation (product)
- Otic preparation (product)
- Oxidized cellulose (product)
- Pesticide product (product)
- Proprietary agent AND/OR biological (product)
- Renal drug (product)
- Replacement preparation (product)
- Reproductive system drug (product)
- Respiratory drugs (product)
- Skin agent (product)
- Throat preparation (product)
- Type of drug preparation (product)
- Vaccine, immunoglobulins and antisera (product)
- Veterinary proprietary drug AND/OR biological (product)
- Vitamin preparation (product)

18,735 drug concepts in SNOMED CT (<10%)





# Drugs in MeSH

MeSH Tree Structures - 2006 - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://www.nlm.nih.gov/cgi/mesh/2006/MB.cgi

## MeSH Tree Structures - 2006

[Return to Entry Page](#)

1. [+](#) Anatomy [A]
2. [+](#) Organisms [B]
3. [+](#) Diseases [C]
4. [+](#) **Chemicals and Drugs [D]**
5. [+](#) Analytical, Diagnostic and Therapeutic Techniques and Equipment [E]
6. [+](#) Psychiatry and Psychology [F]
7. [+](#) Biological Sciences [G]
8. [+](#) Physical Sciences [H]
9. [+](#) Anthropology, Education, Sociology and Social Phenomena [I]
10. [+](#) Technology and Food and Beverages [J]
11. [+](#) Humanities [K]
12. [+](#) Information Science [L]
13. [+](#) Persons [M]
14. [+](#) Health Care [N]
15. [+](#) Publication Characteristics [V]
16. [+](#) Geographic Locations [Z]

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# Drugs in MeSH

## 4. ☐ Chemicals and Drugs [D]

- ◊ [Inorganic Chemicals \[D01\]](#) +
- ◊ [Organic Chemicals \[D02\]](#) +
- ◊ [Heterocyclic Compounds \[D03\]](#) +
- ◊ [Polycyclic Compounds \[D04\]](#) +
- ◊ [Macromolecular Substances \[D05\]](#) +
- ◊ [Hormones, Hormone Substitutes, and Hormone Antagonists \[D06\]](#) +
- ◊ [Enzymes and Coenzymes \[D08\]](#) +
- ◊ [Carbohydrates \[D09\]](#) +
- ◊ [Lipids \[D10\]](#) +
- ◊ [Amino Acids, Peptides, and Proteins \[D12\]](#) +
- ◊ [Nucleic Acids, Nucleotides, and Nucleosides \[D13\]](#) +
- ◊ [Complex Mixtures \[D20\]](#) +
- ◊ [Biological Factors \[D23\]](#) +
- ◊ [Biomedical and Dental Materials \[D25\]](#) +
- ◊ [Pharmaceutical Preparations \[D26\]](#) +
- ◊ [Chemical Actions and Uses \[D27\]](#) +

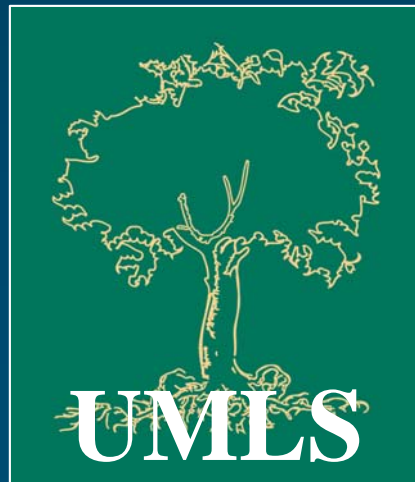
8,140 drug descriptors in MeSH (~30%)





# Drug vocabulary integration

*Unified Medical Language System*





# Source Vocabularies

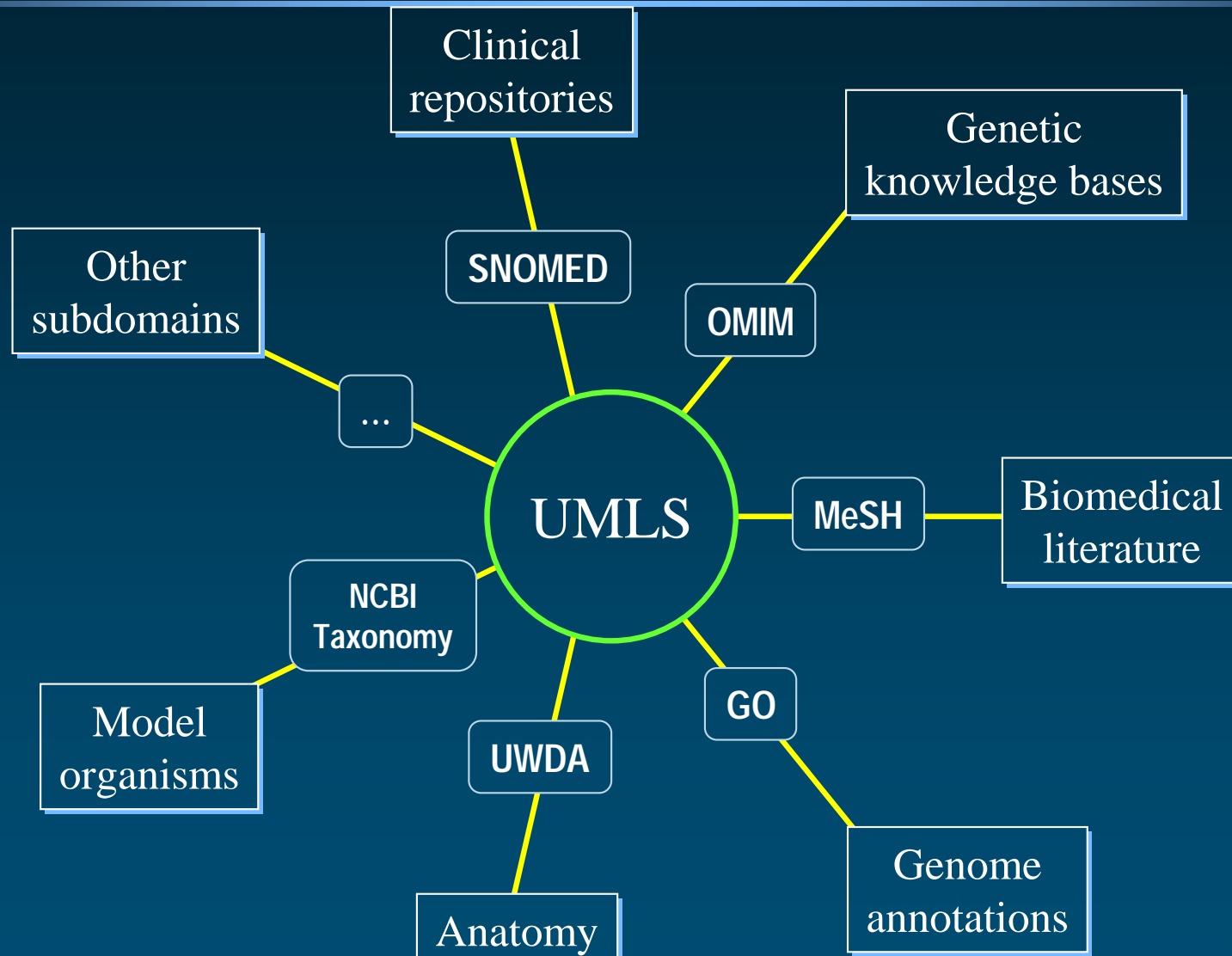
(2006AA)

- ◆ 140 source vocabularies
  - 17 languages
- ◆ Broad coverage of biomedicine
  - 5M names
  - 1.3M concepts
  - 16M relations
- ◆ Common presentation



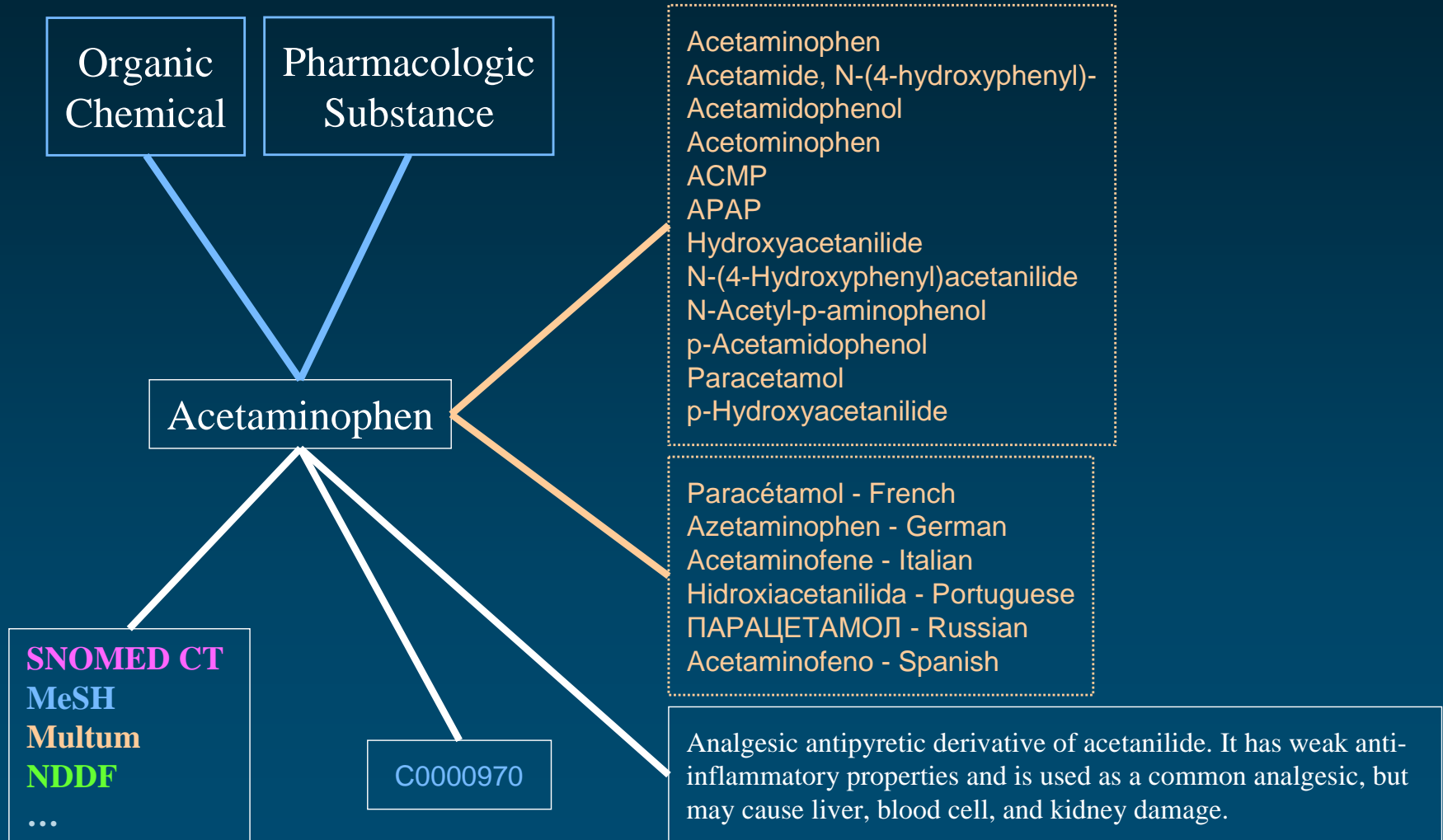


# Integrating subdomains





# Metathesaurus concept





# Metathesaurus drug concepts

## ◆ Semantic types

- Pharmacologic Substance 101,801
  - Antiparkinson Agents
  - Vidarabine Phosphate
- Antibiotic 3,592
  - Kanamycin
- Clinical Drug 165,378
  - Afrin Nose Drops 0.05%
  - Verapamil Oral Tablet [Calan]

270,000 concepts

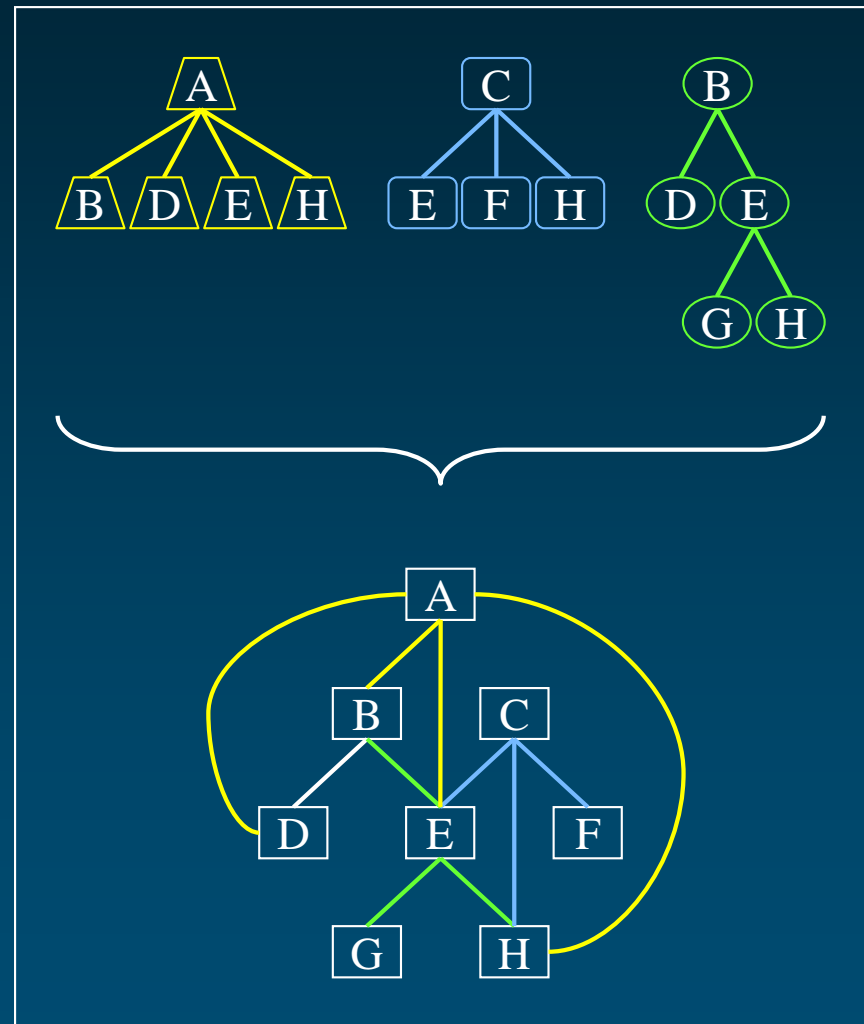
(~21% of all  
Metathesaurus  
concepts)





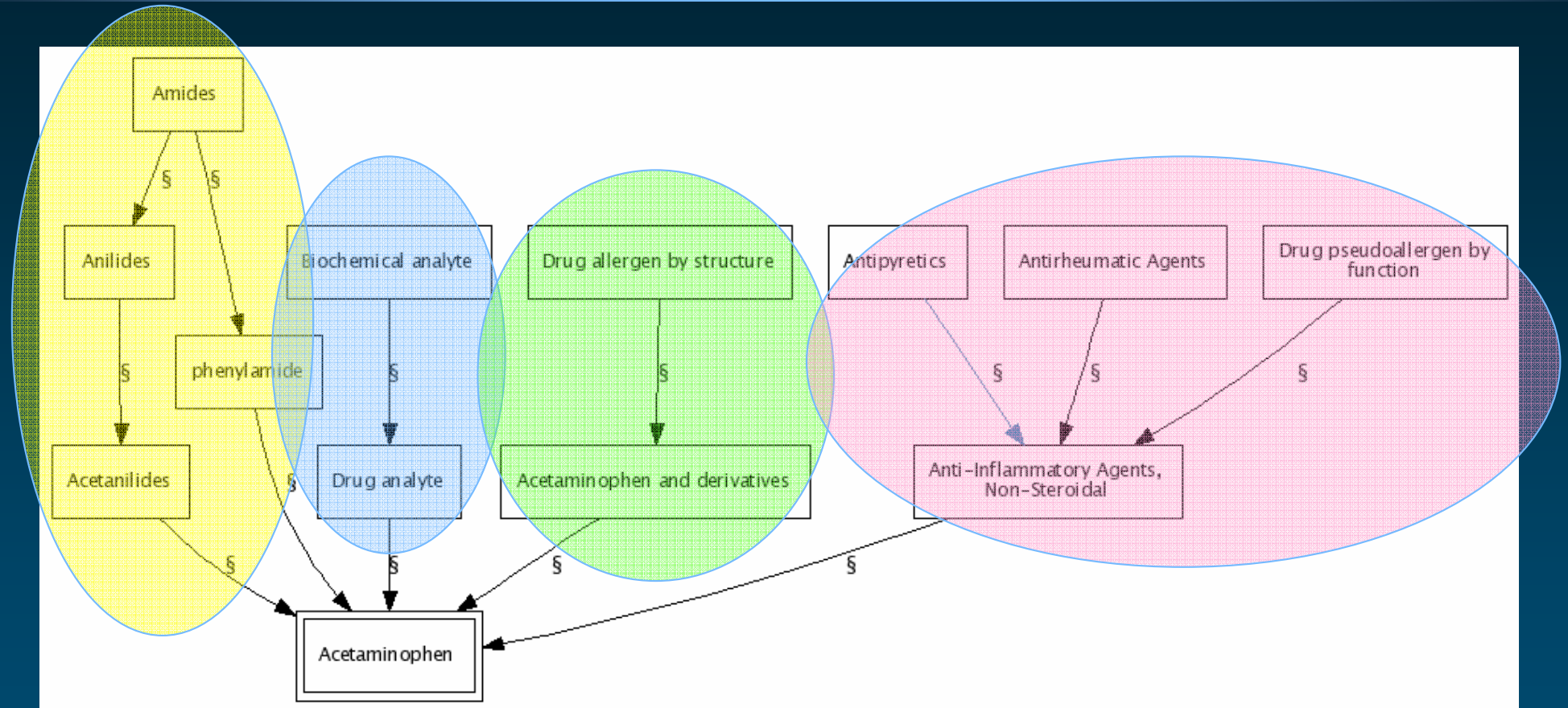
# Organize concepts

- ◆ Inter-concept relationships: hierarchies from the source vocabularies
- ◆ Redundancy: multiple paths
- ◆ One graph instead of multiple trees (multiple inheritance)





# Metathesaurus relations



# Drug vocabulary standardization

*RxNorm*



# Motivation

- ◆ Exchange of information requires standardized names
  - Ordering drugs
  - Checking interactions
  - Inventory management
- ◆ No standard naming conventions for drugs
- ◆ Integrating drug vocabularies
- ◆ Unique identifiers for drugs
- ◆ Specify relations among drug entities



# Normalized form

**Strength**

4mg/ml

**Ingredient**

Fluoxetine

**Dose form**

Oral Solution

**Strength**

Semantic clinical drug component

**Ingredient**

**Ingredient**

**Dose form**

Semantic clinical drug form

**Strength**

Semantic clinical drug

**Ingredient**

**Dose form**



# Generic vs. Brand

## ◆ Generic

- Ingredient (IN) ←
- Clinical drug form (SCDF) ←
- Clinical drug component (SCDC) ←
- Clinical drug (SCD) ←

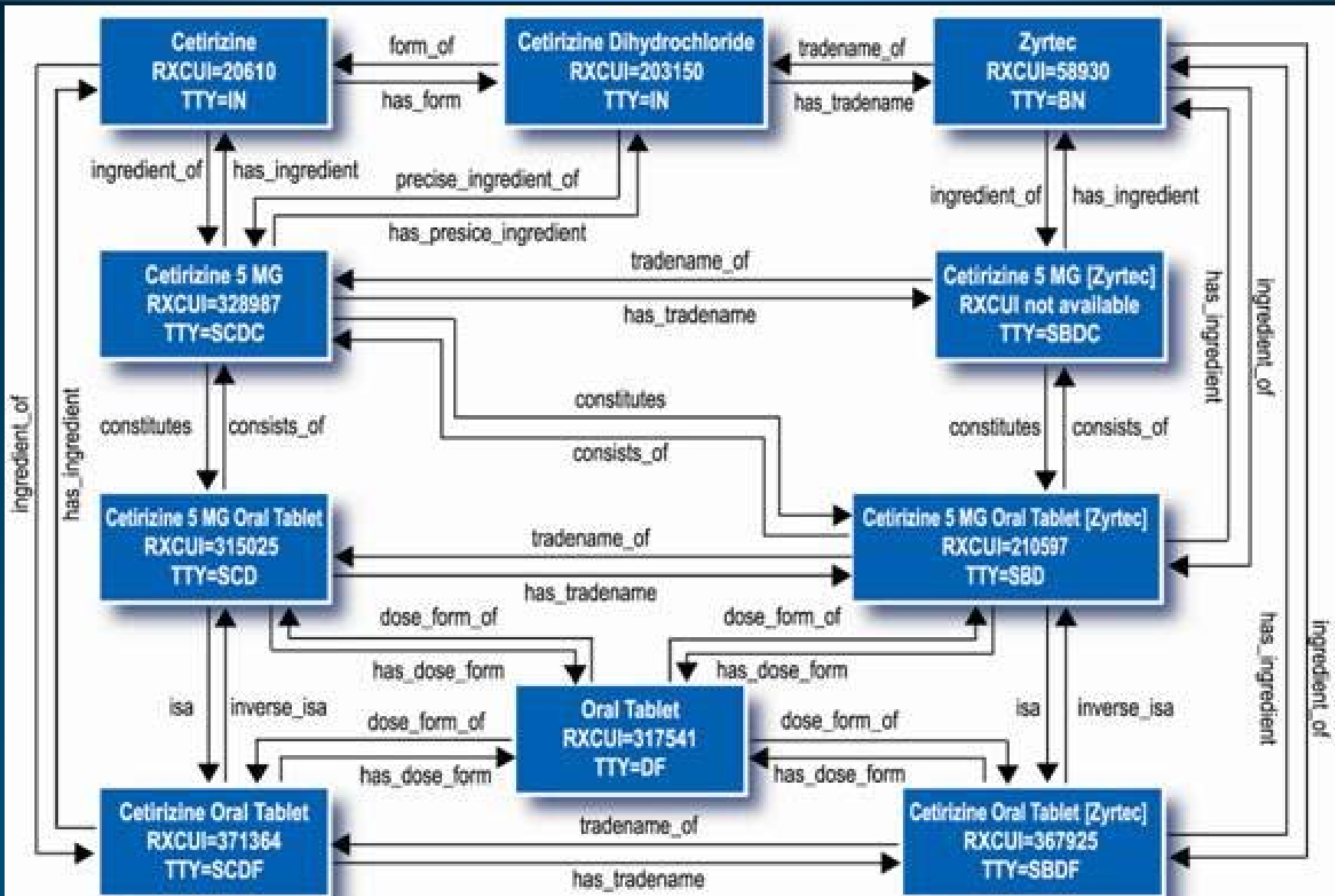
## ◆ Brand

- Brand name (BN)
- Branded drug form (SBDF)
- Branded drug component (SBDC)
- Branded drug (SBD)

*tradename\_of*



# Relations among drug entities



# RxNorm database

## ◆ Data sources

- Master Drug Data Base
- Multum MediSource Lex.
- Micromedex DRUGDEX
- FDA National Drug Code Directory
- National Drug Data File Plus Source Vocabulary
- VA National Drug File
- SNOMED Clinical Terms

## ◆ Content

- 5,570 ingredients
- 10,788 brand names
- 22,724 clinical drug comp.
- 29,734 clinical drugs
- 17,149 branded drugs
- 16,447 branded drug comp.
- 13,516 clinical drug forms
- 13,035 branded drug forms
- 140 dose forms

*(as of February 28, 2006)*



# Visualization and processing of drug information





# RxNav

- ◆ Visualization and navigation
  - RxNorm browser
  - Spelling correction
  - Search on names and codes
  - Standalone application
    - RxNorm database at NLM
    - Local RxNorm database
- ◆ Drug information processing
  - API to the RxNorm database
  - Web services





# RxNav demo

<http://mor.nlm.nih.gov/download/rxnav/>



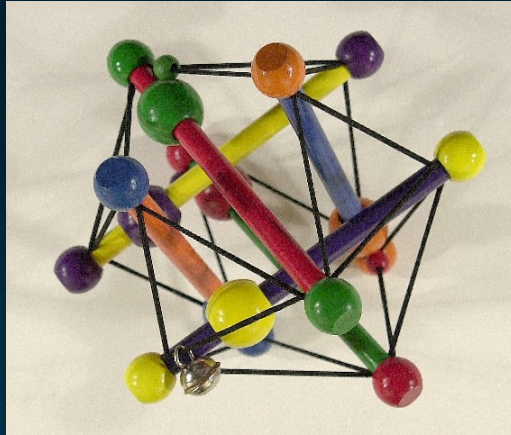


# Conclusions

# Conclusions

- ◆ Biomedical ontology and drug discovery
  - Ontologies provide
    - Terminology for entity recognition (text mining)
    - Relations for reasoning about drugs
  - Terminology integration and standardization (RxNorm) enables interoperability and mapping across vocabularies
    - Entry point into knowledge bases
  - Integration into broad ontologies (UMLS) enables information integration across subdomains





# Medical Ontology Research

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# References

## Drug vocabularies

- MDDDB <http://www.medispan.com/Products/index.aspx?id=1>
- Multum <http://www.multum.com/>
- DRUGDEX <http://www.micromedex.com/products/drugdex/>
- FDA NDC Dir. <http://www.fda.gov/cder/ndc/>
- NDDF Plus [http://www.firstdatabank.com/knowledge\\_bases/nddf\\_plus/](http://www.firstdatabank.com/knowledge_bases/nddf_plus/)

## Other vocabularies

- MeSH <http://www.nlm.nih.gov/mesh/>
- SNOMED CT <http://www.snomed.org/>



# References

## Unified Medical Language System (UMLS)

- <http://www.nlm.nih.gov/research/umls/>
- Bodenreider O. (2004). The Unified Medical Language System (UMLS): Integrating biomedical terminology. *Nucleic Acids Research*; D267-D270.

## RxNorm

- <http://www.nlm.nih.gov/research/umls/rxnorm/index.html>



- <http://mor.nlm.nih.gov/download/rxnav/>

