

Aligning GO with ChEBI

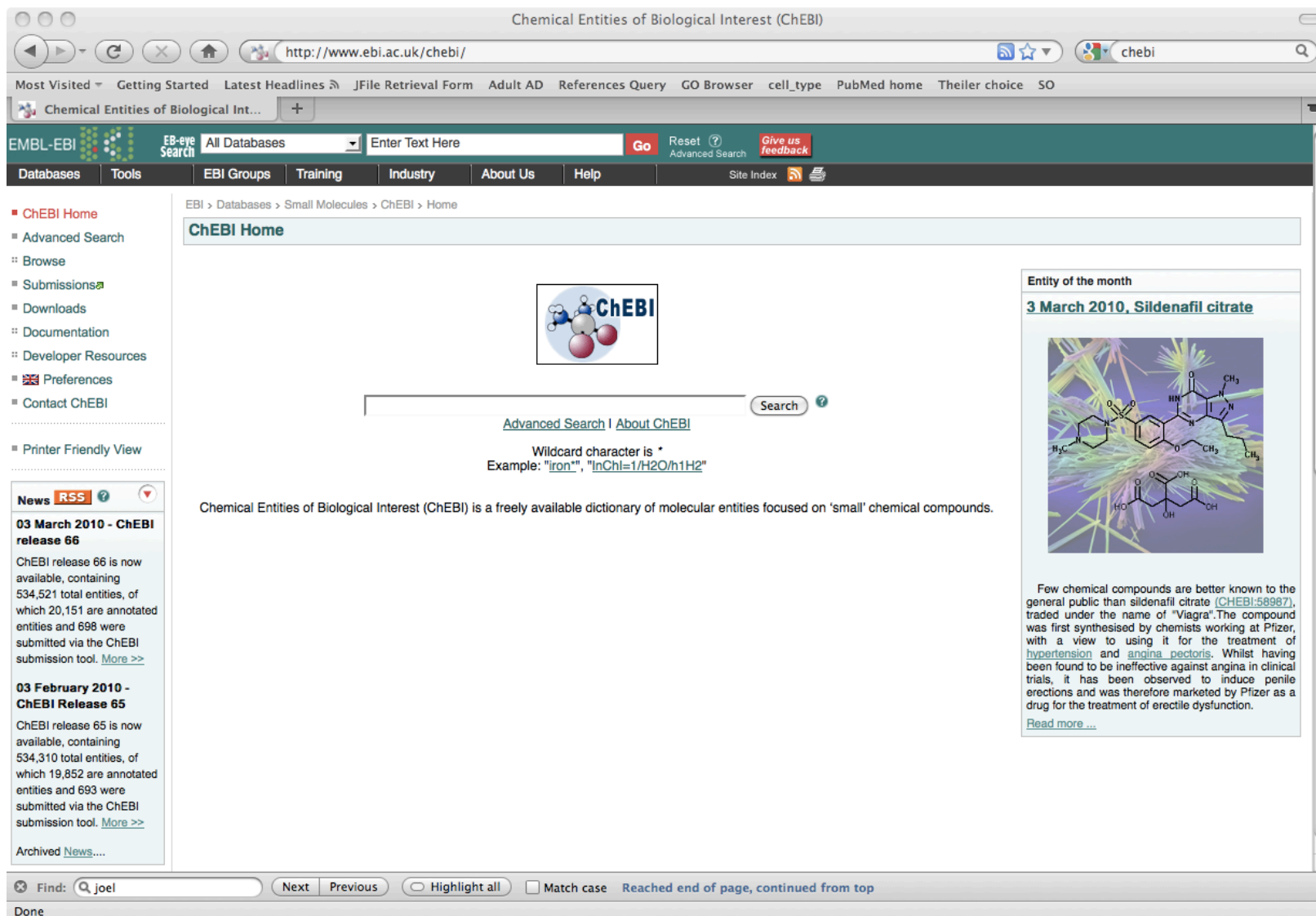
David, Midori, Jane, Tanya, Harold,
Chris

Hopefully you are all convinced that making cross products is a good idea

The first external ontology we will align and make cross-products with is ChEBI

- The GO is littered with chemicals
 - Metabolic process
 - Biosynthetic Process
 - Catabolic Process
 - Transport
 - Transporter Activity
 - Response to Chemical
 - Catalytic activity
 - Binding

The first external ontology we will align and make cross-products with is ChEBI



The screenshot shows the ChEBI website homepage in a browser window. The browser address bar shows the URL <http://www.ebi.ac.uk/chebi/>. The page features a navigation menu with links for Databases, Tools, EBI Groups, Training, Industry, About Us, and Help. A search bar is prominently displayed with the text "Enter Text Here" and a "Go" button. Below the search bar, there are links for "Advanced Search" and "About ChEBI". The main content area includes a "ChEBI Home" heading, a search box, and a description of ChEBI as a freely available dictionary of molecular entities. A sidebar on the left contains a "News" section with RSS feeds for recent releases (March 2010 and February 2010). On the right, there is an "Entity of the month" section for Sildenafil citrate, featuring its chemical structure and a brief history.

Chemical Entities of Biological Interest (ChEBI)

<http://www.ebi.ac.uk/chebi/>

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Chemical Entities of Biological Int...

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ChEBI Home

EBI > Databases > Small Molecules > ChEBI > Home

ChEBI Home

Advanced Search | About ChEBI

Search

Wildcard character is *
Example: "iron", "InCh=1/H2O/h1H2"

Chemical Entities of Biological Interest (ChEBI) is a freely available dictionary of molecular entities focused on 'small' chemical compounds.

Entity of the month
3 March 2010, Sildenafil citrate

Few chemical compounds are better known to the general public than sildenafil citrate (CHEBI:58987), traded under the name of "Viagra". The compound was first synthesised by chemists working at Pfizer, with a view to using it for the treatment of hypertension and angina pectoris. Whilst having been found to be ineffective against angina in clinical trials, it has been observed to induce penile erections and was therefore marketed by Pfizer as a drug for the treatment of erectile dysfunction.

Read more ...

Find: joel Next Previous Highlight all Match case Reached end of page, continued from top

Done

Our first pass at trying to align the chemicals in GO with chemicals in ChEBI pointed out some issues

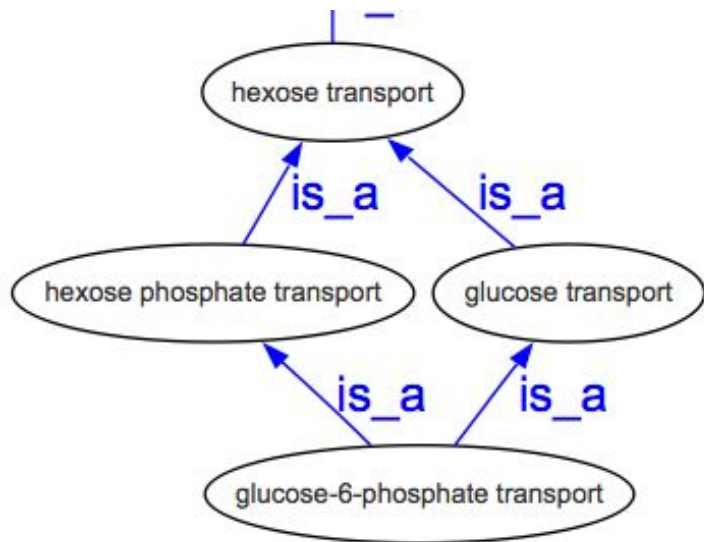
← CHEBI:33243 natural product
↑ Δ CHEBI:23008 carbohydrate
 ↑ Δ CHEBI:26816 carbohydrate phosphate
 ↑ Δ CHEBI:25608 nucleoside phosphate
 ↑ Δ **CHEBI:36976 nucleotide**
 ↑ Δ CHEBI:36981 flavin nucleotide

Is nucleotide biosynthesis a type of carbohydrate biosynthesis?

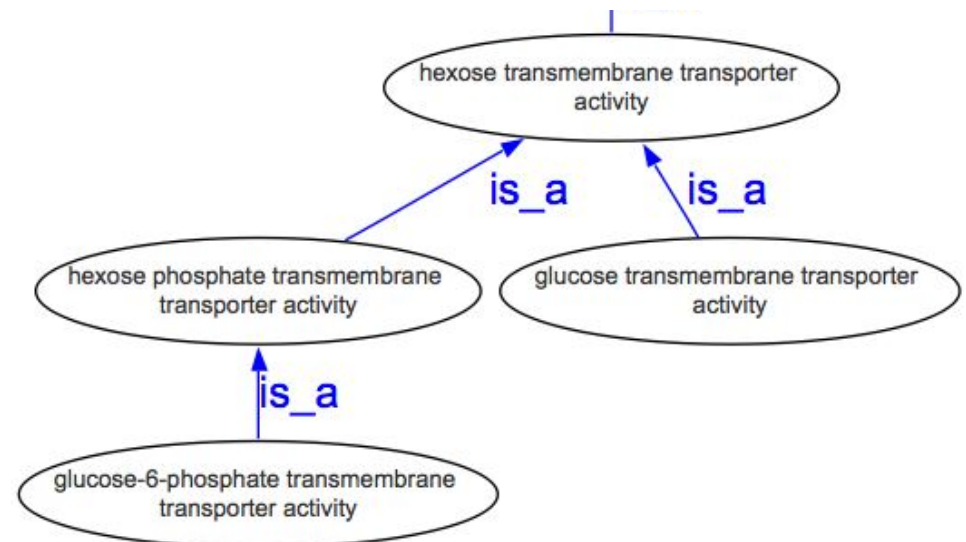
If you are catabolizing the sugar moiety of a glycoprotein, is it protein catabolism?

... Δ CHEBI:33695 information biomacromolecule
 ↑ Δ CHEBI:36080 protein
 ↑ Δ CHEBI:33837 conjugated protein
 ↑ Δ **CHEBI:17089 glycoprotein**
 ↑ Δ CHEBI:37396 proteoglycan

Adding MF-BP links also showed that GO had issues too!

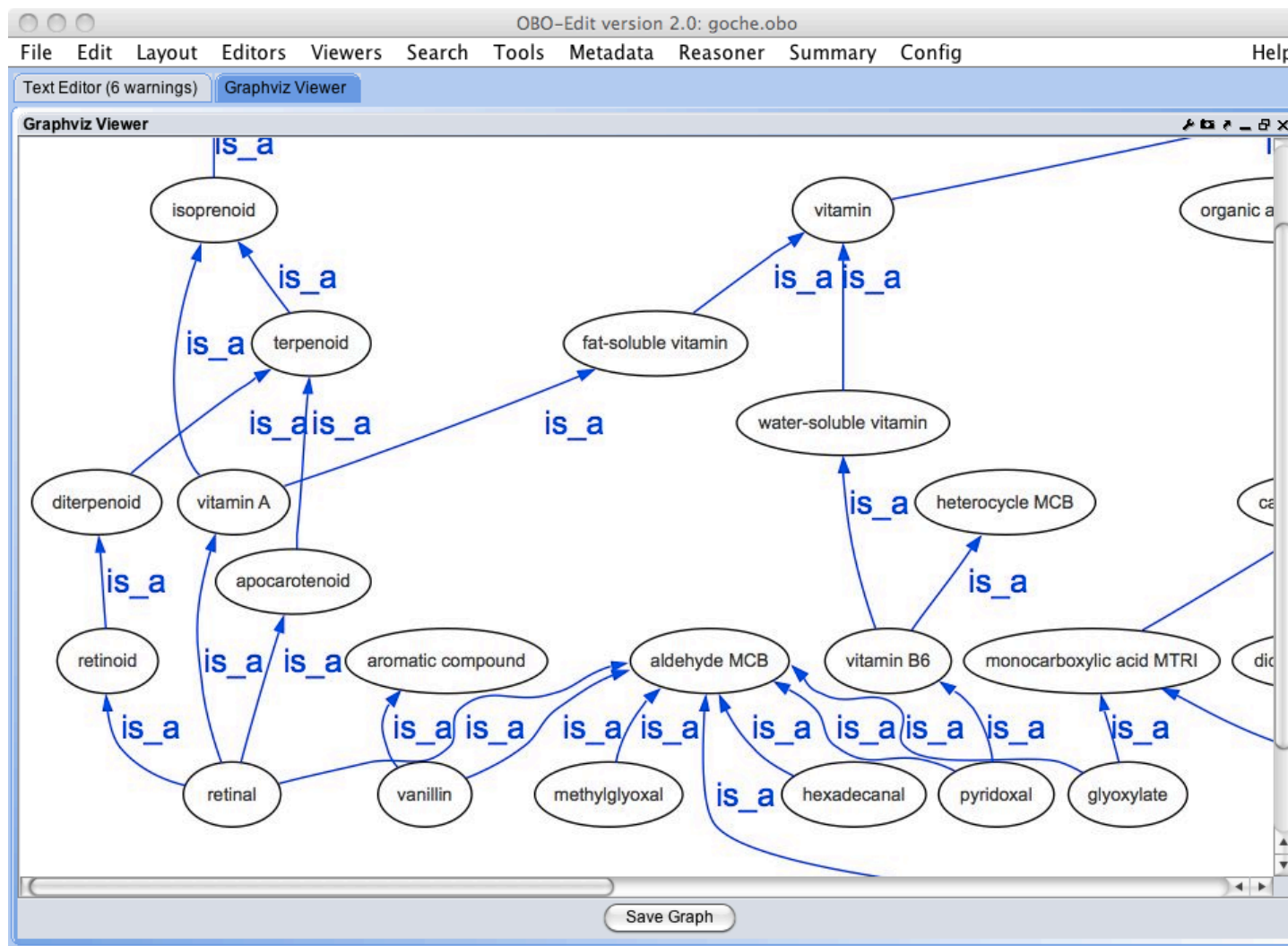


Biological Process



Molecular Function

We decided we needed to get GO in order: The birth of GOChe



Our current goal is to represent the inherent chemical ontology that already exists In GO. Every Tuesday we tag-team work on this file.

GOChe is the representation of chemicals in GO

- If a chemical in GO is also represented in ChEBI, then we take the ChEBI ID for the chemical
- If a chemical is in GO and is not in ChEBI, then the chemical is added with a GOChe_ID to be resolved with ChEBI later.
- GOChe has around a thousand terms
- GOChe represents the union of all of the relationships between chemicals in GO

GOChE Terms

This screenshot shows the 'Text Editor' window for the term 'apocarotenoid'. The window title is 'Text Editor' and it has tabs for 'Text Editor' and 'Graphviz Viewer'. The main content area shows the following fields:

- ID: GOCHE:0090041
- Namespace: chebi_ontology
- Name: apocarotenoid

Below these fields are three tabs: 'Definition *', 'Comment', and 'Cross Products'. The 'Definition *' tab is active, showing a text area with the content 'x.'. To the right of the definition is a 'Dbxrefs' section with a list containing 'GOC:chem_mtg' and two buttons, '+' and '-'.

This screenshot shows the 'Text Editor' window for the term 'pyridoxal'. The window title is 'Text Editor (5 warnings)' and it has tabs for 'Text Editor (5 warnings)' and 'Graphviz Viewer'. The main content area shows the following fields:

- ID: CHEBI:17310
- Secondary IDs: CHEBI:14976, CHEBI:26423, CHEBI:269111, CHEBI:45112, CHEBI:8667
- Namespace: chebi_ontology
- Name: pyridoxal

Below these fields are three tabs: 'Definition *', 'Comment', and 'Cross Products'. The 'Definition *' tab is active, showing a text area with the content 'A vitamin B6 that has formula C8H9NO3.'. To the right of the definition is a 'Dbxrefs' section with a list containing 'GOC:chem_mtg' and two buttons, '+' and '-'.

Plan, part 1

- Finish GOChe as chemicals are represented in GO now
- Refine/correct GOChe once it is complete
 - Create/refine definitions of terms based on GO best practice
- Create cross products for current GO chemical terms
- Refine terms that contain chemical information, but have no chemical parents, for example diazepam.
- Write rules for how GO terms can be used for reasoning. For example, a part_of link in GO should **not** translate into an is_a link in GO CHE
- Internally align GO!

Plan , part 2

- Align GOChE with ChEBI
 - Determine where misalignments occur
- GOChE team-ChEBI team meeting?
 - Discuss the misalignments
 - Come to a consensus on plural terms like ‘phenols’ and compound terms like ‘thiamine and derivative’
 - Come to a consensus on definitions
- Use ChEBI as the external ontology for GO cross-products