Leveraging EMBL-EBI tools in SciBite

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Majority of scientific information is unstructured and underused.

Information overload (Volume, Variety, Velocity, Quality)

Highly synonymous and ambiguous terminology

Complex hierarchical relationships

AI still to deliver major benefits in research
Enterprise Ready Core Technology

SciBite Semantic Platform

- **VOCabs**
- **TERMite**

- Designed for integration
- Modern, Java-based RESTful API
- RDBMS, NOSQL, Solr/Elastic, Hadoop, RDF, AWS & Docker compatible
- Scalable & fast. Runs on a server, cloud, laptop

Text, Documents, Databases

Machine-readable data
The Science

Ontologies are at the heart of everything

Hand curated and maintained by our expert team

Comprehensive coverage

Aligned to industry standards to maintain interoperability

Enriched with synonyms and rules to manage the complexity of scientific language

Customize, augment our existing or deploy your own vocabularies
What Is A Vocab?

Ontology, Taxonomy, List
Public Or Internal

Expert Curation

Machine Curation
(Variation Engine)

Linguistic Rules

TERMite Vocab
EBI chemistry resources
Used to create SciBite DRUG vocab

Enrich with additional synonyms and rules, and supplement with phase 2 & 3 compounds

Feed back to ChEMBL duplicate compounds, errors and new compounds
MetaboLights

Turning compound list into a vocab
Supplement with LIPIDMAPS
Cross-reference to HMDB
The efficiency of compounds of the invention in inhibiting the S. aureus-induced lipid phosphorylation may be tested in the following binding assay. The assay combines the Scintillation Proximity Assay (SPA, Amersham) with the capacity of neomycin to bind phosphorylated lipids with high affinity and specificity. Scintillation Proximity Assay is based on the properties of weakly emitting isotopes (such as 3H, 125I, 32P). Coating SPA beads with neomycin allows the detection of phosphorylated lipid substrates after incubation with recombinant NIH and radioactive ATP in the same well, by capturing the radioactive phospholipids to the SPA beads through their specific binding to neomycin. To a 384 well MTP containing 5 μl of the test compound of Formula (1) (suspended in 2% DMEM) to yield a final concentration of 20, 5, 1.25, 0.3125, 0.0781, 0.0195, 0.004, 0.0013 and 0.0003 μM of the test compound(s), the following assay components are added: 1.5 μl of 50 μM micros 1.25 μl of buffer (33 mM Tris/NaOH pH 7.4, 33 mM MgCl2, 33 mM DTT, 4 mM NaVO4, 0.4 μM Hesperidin, 40 mM pH 7.4) and 3.5 μl of human recombinant GST-CtBP in 2% DMEM (in Hepes, pH 7.4). After incubation at 30°C for 120 minutes with gentle agitation, the reaction is stopped by addition of 60 μl of 1% solution containing 75 μg of neomycin coated PVT SPA beads, ATP 6.5 μM and EDTA 6.5 μM in PBS. The assay is further incubated at room temperature for 60 minutes with gentle agitation to allow binding of phospholipids to neomycin-SPA beads. After precipitation of the neomycin-coated PVT SPA beads for 5 hours, radioactive Phospholipids are quantified by Scintillation counting in a Wallac MicroBeta™ plate counter.

Example 510: Mechanistic on-target cell assay

The cellular activity of the examples was measured by Flow Cytometry assay format using a Ramos B-lymphocyte cell line (AYCC eCRL-1923). These cells were incubated overnight in 5% CO2 and next day treated to reduce background of AKT phosphorylation. Pre-incubated with test compounds for 20 min and then stimulated with anti-human FcγRIIa (OKT 6 clone) (10 ng/ml) for 15 minutes. The reaction was stopped by fixing the cells with Paraformaldehyde 5% (final) for 10 minutes at room temperature. Cells were washed once with Phosphate Buffer Saline (PBS), permabilised in PBS-BenKoX-0.1% for 20 minutes at room temperature washed twice with PBS and once with PBS-0.1% (final) and the cells were stained with a mixture of Mouse anti-human 1μM-APC (BD Pharmingen 555061) (1:50), anti-IgG-FITC Alexa 488 (Invitrogen Re.48-555A) (1:200) and Cito IgG (5μg/ml, 100 ng/mL) (Invivogen, BD Pharmingen 555061) (1:200) for 30 minutes at 4°C. Cells were washed twice in PBS and re-suspended in PBS. The cell suspension was passed on a FC500 Flow cytometer (Becton-Dickinson), gating on the IgG positive cells and measuring the AKT phosphorylation.

Examples of inhibitory activities for compounds according to the invention are set out in Table I below.

Table I
Genes and proteins

UniProt for species-specific vocabs
  e.g. Arabidopsis gene/protein

HGNC for human genes

Experimental factor ontology (EFO) for Transcriptomics

Lots of work tailoring these for text-mining:
  e.g. WAS, PAGE1, SEPT1
EBI Ontology Services
Ontology mapping: OxO

EMBL-EBI Ontology Xref Service

Provides up-to-date mappings between ontologies

Addresses common need to pivot between ontologies

UI and API
SciDB is a database of relationships between entities. Allows traversing between ontologies and entity types. Add known connections from OXO, UniProt-GOA.
Pistoria Alliance Ontology Mapping Project

Phase 3: joint project between Pistoria Alliance and EMBL-EBI

Develop and evaluate technologies to map between phenotype ontologies

Welcome to the EMBL-EBI Ontology Lookup Service.

Search OLS...

Examples: diabetes, GO:0008743

Looking for a particular ontology?

About OLS
The Ontology Lookup Service (OLS) is a repository for biomedical ontologies that aims to provide a single point of access to the latest ontology versions. You can browse the ontologies through the website as well as programmatically via the OLS API. OLS is developed and maintained by the Samples, Phenotypes and Ontologies Team (SPOT) at EMBL-EBI.

Related Tools
In addition to OLS the SPOT team also provides the OxO, Zooma and Webulous services. OxO provides cross-ontology mappings between terms from different ontologies. Zooma is a service to assist in mapping data to ontologies in OLS and Webulous is a tool for building ontologies from spreadsheets.

Contact Us
For feedback, enquiries or suggestions about OLS or to request a new ontology please contact ols-support@ebi.ac.uk. For bugs or problems with the code or API please report on GitHub issue. For announcements relating to OLS, such as new releases and new features sign up to the OLS announce mailing list.