

AUTOMATIC FUNCTIONAL ANNOTATION OF PUBCHEM BIOASSAYS

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BACKGROUND and OBJECTIVES

The PubChem Bioassay collection is a set of 1293 assays that cover a wide range of compounds of different sizes (from 20 molecules to 200,000 molecules), and techniques (enzymatic, phenotypic etc.).

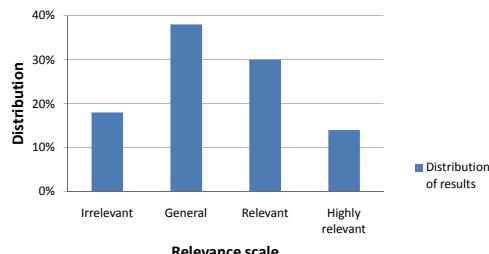
We designed an automated approach to associate each bioassays with a set of functional categories, in order to help search and navigate the assays.

DATA and METHODS

The description section of each assay record was sent to the Gene Ontology Categorizer web services. Designed to help text to GO curation, the categorizer typically outputs a ranked list of GO descriptors.

A sample (size = 30) of the resulting association was manually assessed, using a four-value scale : **highly relevant, relevant, relevant but general, irrelevant**.

RESULTS and NEXT STEPS



1. Relevant assignments massively overcome irrelevant associations: 82% vs 18%.

2. With the availability of formalized annotations, we plan to extend the interface to support more sophisticated similarity based searches as well as more intuitive visualizations of inter-assays relationships.

RESOURCE AVAILABILITIES

The screenshot shows a web-based interface for querying PubChem Bioassay data using GO annotations. The interface includes fields for Assay Selection (with a dropdown menu listing various assay IDs like 590, 581, 583, etc.), GO Term, GO Term Type (checkboxes for Function, Component, Pathway), and GO Term Count (a dropdown menu showing '5'). Below these fields is a 'Perform Query' button. To the right, there is a summary text about the bioassay collection and a table of results. The table has columns for Term, ID, Type, and Score. The first few rows of the table are:

| Term | ID | Type | Score |
|---|---------|------|-------|
| positive regulation of cell proliferation | 0008284 | p1 | 10000 |
| protein amino acid binding | 0005515 | f1 | 8415 |
| negative regulation of cell proliferation | 0008285 | p1 | 5103 |
| negative regulation of cell growth | 0030308 | p1 | 3600 |
| nucleus | 0005634 | c1 | 3413 |

The database and query interface are available at <http://goassay.rguha.net/index.html>
The GO Categorizer is available at <http://eagl.unige.ch/GOCat>