Drug Resource Comparison

ChEMBL, NCATS Inxight Drugs, Open Targets

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Purpose and Approach

Purpose

- Evaluate how comprehensive and authoritative results from each resource appear
- Demonstrate use of drug resource APIs using Python

Approach

- Follow gene target to approved drugs and disease indications
- Investigate gene target ADRB2, approved drug Albuterol, and disease Asthma
- Focus on comparing indications, evidence, and resource activity

Drug Resources: Descriptions and Management (1 of 2)

ChEMBL

- "A manually curated database of bioactive molecules with drug-like properties"
- Managed by European Molecular Biology Laboratory-European Bioinformatics Institute (EMBL-EBI) Chemical Biology Services
- Twenty-four team members supporting four services

NCATS Inxight Drugs

- "A comprehensive portal for drug development information"
- Managed by NCATS/NIH, Division of Preclinical Innovation, IFX Core
- Two team members supporting one service

Drug Resources: Descriptions and Management (2 of 2)

Open Targets Platform

- "A comprehensive tool that supports systematic identification and prioritisation of potential therapeutic drug targets"
- Managed by a consortium of partner institutions including EMBL-EBI, Genentech, GSK, MSD, Pfizer, Sanofi, Wellcome Sanger Institute
- Forty-seven team members supporting one service

Drug Resources: APIs and Example Use (1 of 2)

See springbok-drug-resource-comparison repository

ChEMBL

- API: Data Web Services documentation, Python client repository (not actively developed), and webresource client examples
- Usage: chembl.py [-h] [–gene-symbol GENE_SYMBOL] [-f]
- Performance: Got ChEMBL target data for ADRB2 in 383 s on the first request, and under 3 s on the second request, suggesting the responses are cached

NCATS Inxight Drugs

- API: Inxight (no repository located), and Stitcher (repository archived)
- Usage: ncats.py [-h] [–compound-name COMPOUND_NAME] [-f]
- Performance: Got NCATS GSRS data for ALBUTEROL in 8 s, and Stitcher data for ALBUTEROL in 3 s, although performance varied

Drug Resources: APIs and Example Use (2 of 2)

See springbok-drug-resource-comparison repository

Open Targets Platform

- API: gget (repository actively developed), and Open Targets API Description, GraphQL API, GraphQL API playground, and repository (actively developed)
- Usage: gget_cli.py | open_targets.py [-h] [–gene-symbol GENE_SYMBOL]
- Performance: Got gget data for ADRB2 in 2 s, got Open Targets data for ADRB2, and ALBUTEROL in less than 1 s

But wait ... Why no Albuterol? ... And what's with those EFO terms?

Why no Albuterol?

- Open Targets identifies ADRB2 as the only target for Albuterol, while NCATS Inxight also identifies ADRB1
- ADRB2 and ADRB1 do not appear in the NSForest binary or marker gene results
- Since we search for drugs associated with genes, the search does not find Albuterol

And the EFO terms?

- The Experimental Factor Ontology (EFO) describes many experimental variables in EBI databases
- The EFO serves as the core ontology for Open Targets
- Cross references are provided to many other ontologies, including MONDO

Drug Resources: Results Comparison and Evaluation

Observations and Recommendations