# Drug Resource Comparison

## ChEMBL, NCATS Inxight Drugs, Open Targets

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# Purpose and Approach

## Purpose

- Compare how comprehensive, organized, and accessible 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
- Provide data samples for review, and comment by team members

# 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

# 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

# Why consider Open Targets?

Or, 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 these 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

# ChEMBL API and Example Use

See springbok-drug-resource-comparison repository

**API**: Data Web Services documentation, Python client repository (not actively developed), and webresource client examples

**Usage**: chembl.py [-h] [–gene-symbol GENE_SYMBOL] [-f]

- Get ChEMBL target id for a gene symbol
- Get ChEMBL molecule ids for a target id
- Get drugs and drug indications for all molecule ids
- Get SVG image for a drug

**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

# ChEMBL Activity Data for ADRB2


```
"activity": [
  {
    "action_type": null,
    "activity_comment": null,
    "activity_id": 52694,
    "activity_properties": [],
    "assay_chembl_id": "CHEMBL652493",
    "assay_description": "Binding affinity against adrenergic
        receptor subtype Beta-2 adrenergic receptor using
        [3H]DHA as radioligand",
    "assay_type": "B",
    "assay_variant_accession": null,
    "assay_variant_mutation": null,
    "bao_endpoint": "BAO_0000192",
    "bao_format": "BAO_0000357",
    "bao_label": "single protein format",
    "canonical_smiles": "COc1cccc2c1CC[C@H]1CN(CCn3c(=O)[nH]c4c
        (sc5ccccnc54)c3=O)C[C@@H]21",
    "data_validity_comment": null,
    "data_validity_description": null,
    "document_chembl_id": "CHEMBL1130166",
    "document_journal": "J Med Chem",
    "document_year": 1997,
    "ligand_efficiency": {
        "bei": "12.07",
        "le": "0.23",
        "lle": "2.44",
        "sei": "6.75"
    },
    "molecule_chembl_id": "CHEMBL40650",
    "molecule_pref_name": null,
    "parent_molecule_chembl_id": "CHEMBL40650",
    "pchembl_value": "5.41",
    "potential_duplicate": 0,
    "qudt_units": "http://www.openphacts.org/units/Nanomolar",
    "record_id": 199469,
    "relation": "=",
    "src_id": 1,
    "standard_flag": 1,
    "standard_relation": "=",
    "standard_text_value": null,
    "standard_type": "Ki",
    "standard_units": "nM",
    "standard_upper_value": null,
    "standard_value": "3870.0",
    "target_chembl_id": "CHEMBL210",
    "target_organism": "Homo sapiens",
    "target_pref_name": "Beta-2 adrenergic receptor",
    "target_tax_id": "9606",
    "text_value": null,
    "toid": null,
    "type": "Ki",
    "units": "nM",
    "uo_units": "UO_0000065",
    "upper_value": null,
    "value": "3870.0"
  }
]
```

# ChEMBL Drug Data for Albuterol (1 of 2)


```
{
    "applicants": [
        "Dash Pharmaceuticals Llc A Fully Owned Sub Of
            Natco Pharma Ltd",
    ],
    "atc_classification": [
        {
            "code": "R03AC02",
            "description": "RESPIRATORY SYSTEM: DRUGS FOR
                OBSTRUCTIVE AIRWAY DISEASES: ADRENERGICS,
                INHALANTS: Selective beta-2-adrenoreceptor
                agonist"
        },
    ],
    "availability_type": 1,
    "biotherapeutic": null,
    "black_box": 1,
    "black_box_warning": "1",
    "chirality": 0,
    "drug_type": 1,
    "first_approval": 1981,
    "first_in_class": 0,
    "helm_notation": null,
    "indication_class": "Bronchodilator",
    "max_phase": "4.0",
    "molecule_chembl_id": "CHEMBL714",
    "ob_patent": "7105152",
    "oral": 1,
    "parenteral": 0,
    "prodrug": 0,
    "research_codes": [
        "SCH-13949W",
    ],
    "rule_of_five": 1,
    "sc_patent": "US-7105152-B1",
    "synonyms": [
        "Albuterol sulfate (MI, USAN, USP)",
    ],
    "topical": 1,
    "usan_stem": "-terol",
    "usan_stem_definition": "bronchodilators
        (phenethylamine derivatives)",
    "usan_stem_substem": "-terol(-terol)",
    "usan_year": 1971,
    "withdrawn_flag": "0"
```

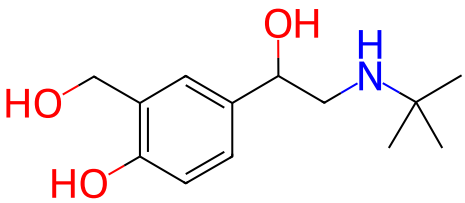
# ChEMBL Drug Data for Albuterol (2 of 2)


```
"molecule_properties": {
    "alogp": "1.31",
    "aromatic_rings": 1,
    "cx_logd": "-1.32",
    "cx_logp": "0.34",
    "cx_most_apka": "10.12",
    "cx_most_bpka": "9.40",
    "full_molformula": "C13H21NO3",
    "full_mwt": "239.31",
    "hba": 4,
    "hba_lipinski": 4,
    "hbd": 4,
    "hbd_lipinski": 4,
    "heavy_atoms": 17,
    "molecular_species": "BASE",
    "mw_freebase": "239.31",
    "mw_monoisotopic": "239.1521",
    "np_likeness_score": "0.56",
    "num_lipinski_ro5_violations": 0,
    "num_ro5_violations": 0,
    "psa": "72.72",
    "qed_weighted": "0.64",
    "ro3_pass": "N",
    "rtb": 4
},
    "molecule_structures": {
        "canonical_smiles": "CC(C)(C)NCC(O)c1ccc(O)c(CO)c1",
        "molfile": "...",
        "standard_inchi": "InChI=1S/C13H21NO3/c1-13(2,3)14-7-
            12(17)9-4-5-11(16)10(6-9)8-15/h4-6,12,14-17H,7-
            8H2,1-3H3",
        "standard_inchi_key": "NDAUXUAQIAJITI-UHFFFAOYSA-N"
    },
    "molecule_synonyms": [
        {
            "molecule_synonym": "Accuneb",
            "syn_type": "OTHER",
            "synonyms": "Accuneb"
        },
    ],
}
```

# ChEMBL Drug Indication Data for Albuterol


```
{
    "drugind_id": 22644,
    "efo_id": "EFO:0000341",
    "efo_term": "chronic obstructive pulmonary disease",
    "indication_refs": [
        {
            "ref_id": "NCT00354354,NCT00358488,NCT00359788,...",
            "ref_type": "ClinicalTrials",
            "ref_url": "https://clinicaltrials.gov/search?term=NCT00354354%20NCT00358488%20NCT00359788%20..."
        },
    ]
    "max_phase_for_ind": "4.0",
    "mesh_heading": "Pulmonary Disease, Chronic Obstructive",
    "mesh_id": "D029424",
    "molecule_chembl_id": "CHEMBL714",
    "parent_molecule_chembl_id": "CHEMBL714"
}
```

# ChEMBL Image for Albuterol



# NCATS Inxight Drugs API and Example Use

See springbok-drug-resource-comparison repository

**API**: Inxight (no repository located), and Stitcher (repository archived)

**Usage**: ncats.py [-h] [–compound-name COMPOUND_NAME] [-f]

- Get GSRS data for a compound unique ingredient identifier
- Get Stitcher data for a compound unique ingredient identifier
- Read Figshare data for a compound unique ingredient identifier
- Decode Figshare conditions field

**Performance**: Got NCATS GSRS data for ALBUTEROL in 8 s, and Stitcher data for ALBUTEROL in 3 s, although performance varied

# NCATS Inxight Drugs GSRS Data for Albuterol


```
{
    "uuid": "7e0fae4c-00c6-4453-a6dc-a60ce10141ae",
    "created": 1743445978000,
    "createdBy": "admin",
    "lastEdited": 1743565750000,
    "lastEditedBy": "admin",
    "deprecated": false,
    "definitionType": "PRIMARY",
    "definitionLevel": "COMPLETE",
    "substanceClass": "chemical",
    "status": "approved",
    "version": "161",
    "approvedBy": "FDA_SRS",
    "names": [...],
    "codes": [...]
    "modifications": {...}
    "notes": [...]
    "properties": [...]
    "approvalID": "QF8SVZ843E",
    "tags": [],
    "structure": {...}
    "moieties": [...]
    "_approvalIDDisplay": "QF8SVZ843E",
    "_name": "ALBUTEROL",
    "access": [],
    "_self": "https://drugs.ncats.io/api/v1/substances(7e0fae4c-00c6-4453-a6dc-a60ce10141ae)?view=full"
}
```

# NCATS Inxight Drugs GSRS Data for Albuterol: Names


```
"names": [
    {
        "uuid": "16e067cd-7fdd-462c-85a6-ac12f53ab4d8",
        "created": 1743445978000,
        "createdBy": "admin",
        "lastEdited": 1743445978000,
        "lastEditedBy": "admin",
        "deprecated": false,
        "name": "1,3-BENZENEDIMETHANOL, .ALPHA.(SUP 1)-(((1,1-DIMETHYLETHYL)AMINO)METHYL)-4-HYDROXY-",
        "type": "cn",
        "domains": [],
        "languages": [
            "en"
        ],
        "nameJurisdiction": [],
        "nameOrgs": [],
        "preferred": false,
        "displayName": false,
        "references": [
            "b6709ca2-68bc-46bd-bd2f-cb333651db46"
        ],
        "access": [],
        "_self": "https://drugs.ncats.io/api/v1/names(16e067cd-7fdd-462c-85a6-ac12f53ab4d8)?view=full"
    },
]
```

# NCATS Inxight Drugs GSRS Data for Albuterol: Codes


```
"codes": [
    {
        "uuid": "1cd3bf3f-6ecd-4a84-8ec7-8a923c037fc8",
        "created": 1743445978000,
        "createdBy": "admin",
        "lastEdited": 1743445978000,
        "lastEditedBy": "admin",
        "deprecated": false,
        "codeSystem": "WHO INTERNATIONAL PHARMACOPEIA",
        "code": "ALBUTEROL",
        "comments": "Description: A white or almost white, crystalline powder; odourless. ...",
        "type": "PRIMARY",
        "url": "http://apps.who.int/phint/pdf/b/Jb.6.1.370.pdf",
        "references": [
            "1545c398-17c3-4d51-a00e-dbcf43cc056a"
        ],
        "access": [],
        "_self": "https://drugs.ncats.io/api/v1/codes(1cd3bf3f-6ecd-4a84-8ec7-8a923c037fc8)?view=full"
    },
]
```

# NCATS Inxight Drugs GSRS Data for Albuterol: Modifications


```
"modifications": {
    "uuid": "d4293ed4-cba3-41cc-8c90-afe244780365",
    "created": 1743445978000,
    "createdBy": "admin",
    "lastEdited": 1743445978000,
    "lastEditedBy": "admin",
    "deprecated": false,
    "agentModifications": [],
    "physicalModifications": [],
    "structuralModifications": [],
    "references": [],
    "access": []
},
```

# NCATS Inxight Drugs GSRS Data for Albuterol: Notes


```
"notes": [
    {
        "uuid": "0b661db6-7f4c-431e-88c5-72d89cb8144d",
        "created": 1743445978000,
        "createdBy": "admin",
        "lastEdited": 1743445978000,
        "lastEditedBy": "admin",
        "deprecated": false,
        "note": "[Validation]WARNING:Code 'QR03AK04'[WHO-VATC] collides (possible duplicate)
            with existing code & codeSystem for substance:\n[Q2WXR1I0PK]CROMOLYN SODIUM",
        "references": [
            "cc331491-ef4a-48c3-9e93-30c9d33aac9a"
        ],
        "access": [
            "admin"
        ]
    },
]
```

# NCATS Inxight Drugs GSRS Data for Albuterol: Properties


```
"properties": [
    {
        "uuid": "3996b30a-6ff4-47c6-9b94-4dc364d75960",
        "created": 1743445978000,
        "createdBy": "admin",
        "lastEdited": 1743445978000,
        "lastEditedBy": "admin",
        "deprecated": false,
        "name": "Volume of Distribution",
        "propertyType": "PHARMACOKINETIC",
        "value": {
            "uuid": "cb7ae50b-e777-4eb3-a349-809e4610b997",
            "created": 1743445978000,
            "createdBy": "admin",
            "lastEdited": 1743445978000,
            "lastEditedBy": "admin",
            "deprecated": false,
            "average": 3.4,
            "units": "Liters/Kilogram",
            "references": [],
            "access": []
        },
        "defining": false,
        "parameters": [],
        "references": [
            "b6340555-7138-c54c-c98f-2f086ba11246"
        ],
        "access": []
    },
]
```

# NCATS Inxight Drugs GSRS Data for Albuterol: Structure


```
"structure": {
    "id": "5a129248-bc18-4545-99a1-5d175834c363",
    "created": 1743445978000,
    "lastEdited": 1743445978000,
    "deprecated": false,
    "digest": "0dc449888fa8e42de5c7e5f7b60941364bfadb55",
    "molfile": "...",
    "smiles": "CC(C)(C)NCC(O)C1=CC(CO)=C(O)C=C1",
    "formula": "C13H21NO3",
    "opticalActivity": "( + / - )",
    "atropisomerism": "No",
    "stereoCenters": 1,
    "definedStereo": 0,
    "ezCenters": 0,
    "charge": 0,
    "mwt": 239.3107,
    "count": 1,
    "createdBy": "admin",
    "lastEditedBy": "admin",
    "hash": "RJYZJCG7HWL2",
    "self": "https://drugs.ncats.io/api/v1/structures
        (5a129248-bc18-4545-99a1-5d175834c363)?view=full",
    "stereochemistry": "RACEMIC",
    "references": [
        "42aba274-8264-4ecf-a4a0-59adad9b98c6",
        "0b8676bd-1f66-4f1f-9737-97a3e13a2d31",
        "82199cff-aff9-4ca9-9948-baf170553652"
    ],
    "access": []
},
```

# NCATS Inxight Drugs GSRS Data for Albuterol: Moieties


```
"moieties": [
    {
        "uuid": "75edf16e-1c0b-4ba3-aa75-5985d23c30b0",
        "created": 1743445979000,
        "createdBy": "admin",
        "lastEdited": 1743445979000,
        "lastEditedBy": "admin",
        "deprecated": false,
        "id": "75edf16e-1c0b-4ba3-aa75-5985d23c30b0",
        "digest": "036ea932aac80052cab2f56f97d446eb52ebbf6d",
        "molfile": "...",
        "smiles": "CC(C)(C)NCC(O)C1=CC(CO)=C(O)C=C1",
        "formula": "C13H21NO3",
        "opticalActivity": "( + / - )",
        "atropisomerism": "No",
        "stereoCenters": 1,
        "definedStereo": 0,
        "ezCenters": 0,
        "charge": 0,
        "mwt": 239.3107,
        "count": 1,
        "hash": "RJYZJCG7HWL2",
        "self": "https://drugs.ncats.io/api/v1/structures
            (75edf16e-1c0b-4ba3-aa75-5985d23c30b0)?view=full",
        "stereochemistry": "RACEMIC",
        "references": [],
        "access": [],
        "countAmount": {
            "uuid": "1b01d0ee-8b2d-4b14-9b7e-2e4fd65f8ae9",
            "created": 1743445979000,
            "createdBy": "admin",
            "lastEdited": 1743445979000,
            "lastEditedBy": "admin",
            "deprecated": false,
            "type": "MOL RATIO",
            "average": 1.0,
            "units": "MOL RATIO",
            "references": [],
            "access": []
        }
    }
]
}
```

# NCATS Inxight Drugs Stitcher Data for Albuterol: PubMed (1 of 2)


```
{
    "name": "PubMed",
    "value": {
        "uid": "14657817",
        "pubdate": "2003 Dec",
        "epubdate": "",
        "source": "J Pediatr",
        "authors": [
            {
                "name": "Carl JC",
                "authtype": "Author",
                "clusterid": ""
            },
        ],
        "lastauthor": "Kercsmar CM",
        "title": "Comparison of racemic albuterol and
            levalbuterol for treatment of acute asthma.",
        "sorttitle": "comparison of racemic albuterol and
            levalbuterol for treatment of acute asthma",
        "volume": "143",
        "issue": "6",
        "pages": "731-6",
        "lang": [
            "eng"
        ],
        "nlmuniqueid": "0375410",
        "issn": "0022-3476",
        "essn": "",
        "pubtype": [
            "Clinical Trial",
            "Journal Article",
            "Randomized Controlled Trial"
        ],
        "recordstatus": "PubMed - indexed for MEDLINE",
        "pubstatus": "4",
        "articleids": [
            {
                "idtype": "pubmed",
                "idtypen": 1,
                "value": "14657817"
            },
        ],
        "history": [
            {
                "pubstatus": "pubmed",
                "date": "2003/12/06 05:00"
            },
        ],
```

# NCATS Inxight Drugs Stitcher Data for Albuterol: PubMed (2 of 2)


```
"references": [
    {
        "refsource": "J Pediatr. 2003 Dec;143(6):702-4.
            doi: 10.1016/j.jpeds.2003.10.018.",
        "reftype": "Comment in",
        "pmid": 14657810,
        "note": ""
    },
],
"attributes": [
    "Has Abstract"
],
"pmcrefcount": "",
"fulljournalname": "The Journal of pediatrics",
        "elocationid": "",
        "doctype": "citation",
        "srccontriblist": [],
        "booktitle": "",
        "medium": "",
        "edition": "",
        "publisherlocation": "",
        "publishername": "",
        "srcdate": "",
        "reportnumber": "",
        "availablefromurl": "",
        "locationlabel": "",
        "doccontriblist": [],
        "docdate": "",
        "bookname": "",
        "chapter": "",
        "sortpubdate": "2003/12/01 00:00",
        "sortfirstauthor": "Carl JC",
        "vernaculartitle": ""
    }
},
```

# NCATS Inxight Drugs Stitcher Data for Albuterol: Description and Phase


```
{
    "value": {
        "description": "Levalbuterol is the (R)-enantiomer of the drug substance racemic albuterol
             (salbutamol). Binding studies have demonstrated that (R)-albuterol binds to the beta2-adrenergic
             receptor with a high affinity, whereas (S)-albuterol binds with 100-fold less affinity than
             (R)-albuterol. Other evaluations have suggested that (R)-albuterol possesses the bronchodilatory,
             bronchoprotective, and ciliary-stimulatory properties of racemic albuterol, while (S)-albuterol
             does not beneficially to the therapeutic effects of the racemate and was originally assumed
             to be inert. Xopenex (levalbuterol HCl) Inhalation Solution is indicated for the treatment
             or prevention of bronchospasm in adults, adolescents, and children 6 years of age and older
             with reversible obstructive airway disease.",
        "uri": [
            "https://www.accessdata.fda.gov/drugsatfda_docs/label/2012/020837s036lbl.pdf |
                https://www.ncbi.nlm.nih.gov/pubmed/15293593 |
                https://www.ncbi.nlm.nih.gov/pubmed/10452786"
        ]
    },
    "name": "Description"
},
{
    "value": {
        "highestPhase": "Approved"
    },
    "name": "Stitcher Highest Phase"
},
```

# NCATS Inxight Drugs Stitcher Data for Albuterol: Targets and Conditions


```
{
    "name": "Targets"
    "value": {
        "StitcherId": "17288.0",
        "id": "CHEMBL210",
        "label": "Beta-2 adrenergic receptor",
        "type": "ChEMBL",
        "pharmacology": "Agonist",
        "potencyType": "Kd",
        "potencyValue": "236.0",
        "potencyDimensions": "nM",
        "potencyUri": "https://www.ncbi.nlm.nih.gov/pubmed/8866170",
        "uri": [
            "https://www.accessdata.fda.gov/drugsatfda_docs/label/
                2012/020837s036lbl.pdf"
        ],
        "condition_refs": null,
        "conditions": []
    },
}
```

```
{
    "name": "Conditions"
    "value": {
        "StitcherId": "17648.0",
        "label": "Asthma",
        "uri": [
            "https://www.ncbi.nlm.nih.gov/pubmed/15293593 ",
            "http://adisinsight.springer.com/drugs/800005434"
        ],
        "highestPhase": "Approved",
        "highestPhaseUri": "https://www.accessdata.fda.gov/
            scripts/cder/ob/results_product.cfm?
            Appl_Type=N&Appl_No=020837",
        "modality": "Primary",
        "productName": "XOPENEX",
        "productFDAUse": "XOPENEX (levalbuterol HCl) Inhalation
            Solution Concentrate is indicated for the treatment
            or prevention of bronchospasm in adults, ...",
        "productFDAUseUri": "https://www.accessdata.fda.gov/
            drugsatfda_docs/label/2012/020837s036lbl.pdf",
        "productDate": "9.2231998E11",
        "isHighestPhaseApproved": "true",
        "approvalSource": "RANCHO",
        "target_refs": null,
        "targets": []
    },
}
```

# NCATS Inxight Drugs FigShare Conditions for Albuterol


```
"condition_id": 17648,
"name": "Asthma",
"condition_uri": "https://www.ncbi.nlm.nih.gov/pubmed/15293593 | ...",
"condition_comment": " ",
"product_name": "XOPENEX",
"product_date": 922320000000,
"condition_highest_phase": "Approved",
"highest_phase_uri": "https://www.accessdata.fda.gov/scripts/cder/ob/results_product.cfm?...",
"fda_use": "XOPENEX (levalbuterol HCl) Inhalation Solution Concentrate is indicated for the
    treatment or prevention of bronchospasm in adults, adolescents, and children 6 years of
    age and older with reversible obstructive airway disease.",
"offlabel_use": "Unknown",
"offlabel_use_uri": "Unknown",
"offlabel_use_comment": " ",
"clinical_trial": "NCT00667797",
"condition_treatment_modality": "Primary",
"condition_do_imprecise": false,
"condition_mesh_imprecise": false,
"mesh_id": "D001249",
"mesh_label": "Asthma",
"do_id": "2841",
"do_label": "asthma",
"is_fda_use": true,
"fda_use_uri": "https://www.accessdata.fda.gov/drugsatfda_docs/label/2012/020837s036lbl.pdf",
"is_product_manual": false,
"highest_phase_discontinued": false,
"product_discontinued": false,
"is_product_date_unknown": false
```

# Open Targets Platform API and Example Use

See springbok-drug-resource-comparison repository

**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]

- Find targets associated with a specific disease or phenotype
- Find diseases and phenotypes associated with a specific target
- Explore evidence that supports a specific target-disease association
- Find tractability and safety information for a specific target
- Find clinical signs and symptoms for a specific disease
- GWAS studies associated with a specified disease
- Find indications for a specific drug
- Credible sets from quantitative trait loci associated with molecular traits containing a specified variant
- Information about a specified study
- Colocalisation metrics for overlapping credible sets from GWAS studies

**Performance**: Got gget data for ADRB2 in 2 s, got Open Targets data for ADRB2, and ALBUTEROL in less than 1 s

# Open Targets: Targets associated with a disease


```
"disease": {
    "id": "MONDO_0004979",
    "name": "asthma",
    "associatedTargets": {
        "count": 3039,
        "rows": [
            {
                "target": {
                    "id": "ENSG00000169252",
                    "approvedSymbol": "ADRB2"
                },
                "score": 0.6148856746523589
            },
        ]
    }
}
```

# Open Targets: Diseases associated with a target


```
"target": {
    "id": "ENSG00000169252",
    "approvedSymbol": "ADRB2",
    "associatedDiseases": {
        "count": 829,
        "rows": [
            {
                "disease": {
                    "id": "MONDO_0004979",
                    "name": "asthma"
                },
                "datasourceScores": [
                    {
                        "id": "chembl",
                        "score": 0.9988218092809733
                    },
                ]
            },
        ]
    }
}
```

# Open Targets: Evidence for target-disease association


```
"disease": {
    "id": "MONDO_0004979",
    "name": "asthma",
    "evidences": {
        "count": 917,
        "rows": [
            {
                "disease": {
                    "id": "MONDO_0004979",
                    "name": "asthma"
                },
                "diseaseFromSource": "bronchospasm",
                "target": {
                    "id": "ENSG00000169252",
                    "approvedSymbol": "ADRB2"
                },
                "mutatedSamples": null,
                "resourceScore": null,
                "significantDriverMethods": null,
                "cohortId": null,
                "cohortShortName": null,
                "cohortDescription": null
            },
        ]
    }
}
```

# Open Targets: Tractability and safety information for a target


```
"target": {
    "id": "ENSG00000169252",
    "approvedSymbol": "ADRB2",
    "tractability": [
        {
            "modality": "SM",
            "label": "Approved Drug",
            "value": true
        },
    ],
```

```
"safetyLiabilities": [
    {
        "event": "cardiac contractility",
        "eventId": "GO_0045823",
        "biosamples": [
            {
                "cellFormat": null,
                "cellLabel": null,
                "tissueLabel": "cardiovascular system",
                "tissueId": "UBERON_0004535"
            }
        ],
        "effects": [
            {
                "dosing": "general",
                "direction": "Activation/Increase/Upregulation"
            }
        ],
        "studies": null,
        "datasource": "Urban et al. (2012)",
        "literature": null
    },
]
}
```

# Open Targets: Clinical signs and symptoms for a disease


```
"disease": {
    "id": "MONDO_0004979",
    "name": "asthma",
    "phenotypes": {
        "count": 5,
        "rows": [
            {
                "phenotypeHPO": {
                    "id": "HP_0032933",
                    "name": "Airway hyperresponsiveness",
                    "description": "An increased sensitivity of
                        the airways to an inhaled constrictor agonist,
                        a steeper slope of the dose-response curve,
                        and a greater maximal response to the agonist.",
                    "namespace": null
                },
                "phenotypeEFO": null,
                "evidence": [
                    {
                        "aspect": "P",
                        "bioCuration": "HPO:probinson[2022-04-15]",
                        "diseaseFromSourceId": "OMIM:600807",
                        "diseaseFromSource": "Asthma, susceptibility to",
                        "evidenceType": "TAS",
                        "frequency": null,
                        "frequencyHPO": null,
                        "qualifierNot": false,
                        "onset": [],
                        "modifiers": [],
                        "references": [
                            "OMIM:600807"
                        ],
                        "sex": null,
                        "resource": "HPO"
                    }
                ]
            },
        ]
    }
}
```

# Open Targets: GWAS studies associated with a disease

diseaseId: MONDO_0004979


```
"studies": {
    "count": 175,
    "rows": [
        {
            "id": "GCST90255360",
            "projectId": "GCST",
            "traitFromSource": "Asthma",
            "publicationFirstAuthor": "Do AR",
            "publicationDate": "2022-12-21",
            "publicationJournal": "Sci Rep",
            "nSamples": 6737,
            "cohorts": [
                "NR"
            ],
            "pubmedId": "36543808",
            "ldPopulationStructure": [
                {
                    "ldPopulation": "eas",
                    "relativeSampleSize": 1
                }
            ]
        },
    ]
}
```

# Open Targets: Indications for a drug


```
"drug": {
    "name": "ALBUTEROL",
    "id": "CHEMBL714",
    "isApproved": true,
    "indications": {
        "count": 35,
        "rows": [
            {
                "maxPhaseForIndication": 4,
                "references": [
                    {
                        "source": "DailyMed",
                        "ids": [
                            "29d24a6d-f9c1-4300-97c7-fec26bdbc22b"
                        ]
                    }
                ],
                "disease": {
                    "id": "MONDO_0004979",
                    "name": "asthma",
                    "dbXRefs": [
                        "ICD9:493.81",
                        "UMLS:C0004096",
                        "DOID:2841",
                        "ICD9:493.9",
                        "ICD9:493",
                        "NCIT:C28397",
                        "icd11.foundation:1656445230",
                        "MESH:D001249",
                        "SCTID:31387002",
                        "HP:0002099",
                        "ICD10CM:J45",
                        "MEDGEN:2109"
                    ],
                    "literatureOcurrences": {
                        "count": 32368,
                        "rows": [
                            {
                                "pmid": "25671117",
                                "pmcid": "PMC4323120",
                                "publicationDate": "2015-01-01"
                            },
                        ]
                    }
                }
            },
        ]
    }
}
```

# Open Targets: Credible sets from quantitative trait loci associated with molecular traits containing a variant


```
"variant": {
    "id": "1_152312600_CACTG_C",
    "qtlCredibleSets": {
        "count": 1,
        "rows": [
            {
                "studyLocusId":
                    "4fea74b7dcc65149b658a71b5c5fa0f3",
                "pValueMantissa": 3.322999954223633,
                "pValueExponent": -7,
                "beta": -0.839744,
                "finemappingMethod": "SuSie",
                "confidence":
                    "SuSiE fine-mapped credible set
                    with in-sample LD",
                "variant": {
                    "id": "1_152057072_G_A",
                    "chromosome": "1"
                },
```

```
            }
        ]
    }
}
```

```
"study": {
    "id": "gtex_exon_stomach_ensg00000143376_14_1_151693484_151693543",
    "studyType": "eqtl",
    "condition": "naive",
    "target": {
        "id": "ENSG00000143376",
        "approvedSymbol": "SNX27"
    },
    "biosample": {
        "biosampleId": "UBERON_0000945",
        "biosampleName": "stomach"
    }
},
"locus": {
    "count": 0,
    "rows": null
},
"locusSize": {
    "count": 2
}
```

# Open Targets: Information about a study


```
"studies": {
    "count": 1,
    "rows": [
        {
            "id": "gtex_exon_stomach_ensg00000143376_14_1_151693484_151693543",
            "studyType": "eqtl",
            "traitFromSource": "ENSG00000143376.14_1_151693484_151693543",
            "projectId": "GTEx",
            "diseases": [],
            "publicationFirstAuthor": null,
            "publicationDate": null,
            "publicationJournal": null,
            "pubmedId": "32913098",
            "nSamples": 324,
            "cohorts": null,
            "ldPopulationStructure": null
        }
    ]
}
```

# Open Targets: Colocalisation metrics for overlapping credible sets

studyLocusId: 4fea74b7dcc65149b658a71b5c5fa0f3


```
"credibleSet": {
    "colocalisation": {
        "count": 18,
        "rows": [
            {
                "otherStudyLocus": {
                    "studyLocusId":
                        "d3ef302b201c3fbc4fc972ebfe4fad0b",
                    "study": {
                        "id": "FINNGEN_R12_L12_FOODDERMAT",
                        "projectId": "FINNGEN_R12",
                        "traitFromSource":
                            "Dermatitis due to ingested food",
                        "publicationFirstAuthor": null
                    },
                    "variant": {
                        "id": "1_152312600_CACTG_C",
                        "chromosome": "1",
                        "position": 152312600,
                        "referenceAllele": "CACTG",
                        "alternateAllele": "C"
                    },
                    "pValueMantissa": 2.427999973297119,
                    "pValueExponent": -8
                },
                "numberColocalisingVariants": 1,
                "colocalisationMethod": "COLOC",
                "h3": 0.005138319255541063,
                "h4": 0.9944360622406548,
                "clpp": null,
                "betaRatioSignAverage": -1
            },
        ]
    }
}
```

# Observations and Next Step

Open Targets appears to offer the most comprehensive resource

- Includes ChEMBL indications data
- Like NCATS Inxight Drugs, includes PubMed and PubMed Central data
- Includes GWAS data

Open Targets data appears well organized, and easily accessible using GraphQL

Open Targets is supported by the largest team, and appears to be actively developed

Next step for team: review and select data elements from each resource here