

GSRS Development Update

5 December 2017

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NIH/NCATS

NCATS

GSRS Status





High level status

- GSRS 2.0 deployed at FDA
 - Enhanced searches
 - Simplified entry forms
 - Scheduled tasks
 - Enhanced export support
 - Bug fixes
- GSRS 2.1 development
 - Bug fixes
 - SDF data import
 - Support for large Nucleic Acids
 - UI simplification
 - Complex facet and filter searches

GSRS Status

High level GSRS Core status

- GSRS 2.1 development (continued)
 - Improved Developer Documentation
 - Much simpler to add customized searches, triggers, and scheduled tasks

 How To Write a Scheduled Task.docx	Refactored scheduled tasks to use simpler in
 How To Write an Entity Processor.docx	Added some more docs
 How To Write an Index Value Maker.docx	Added some more docs
 SubstanceExporterHowTo.md	starting docs folder

GSRS Status

High level GSRS Core status

- GSRS 2.X development
 - Group 3 and Group 4 substance forms and models in testing
 - Porting certain FDA-enhancements to core code

GSRS Status

Issues and Lessons Learned

- Admin and power users often need functionality not built into the UI quickly
 - Turn around time for enhancement to FDA production can be a bottle-neck
 - For many specific tasks, REST API can be used directly
 - Javascript macros
 - Excel Add-on

GSRS Status

GSRS adaptation and customization

- NCATS internal registration system
- FDA GSRS instance
- **Inxight Drugs**

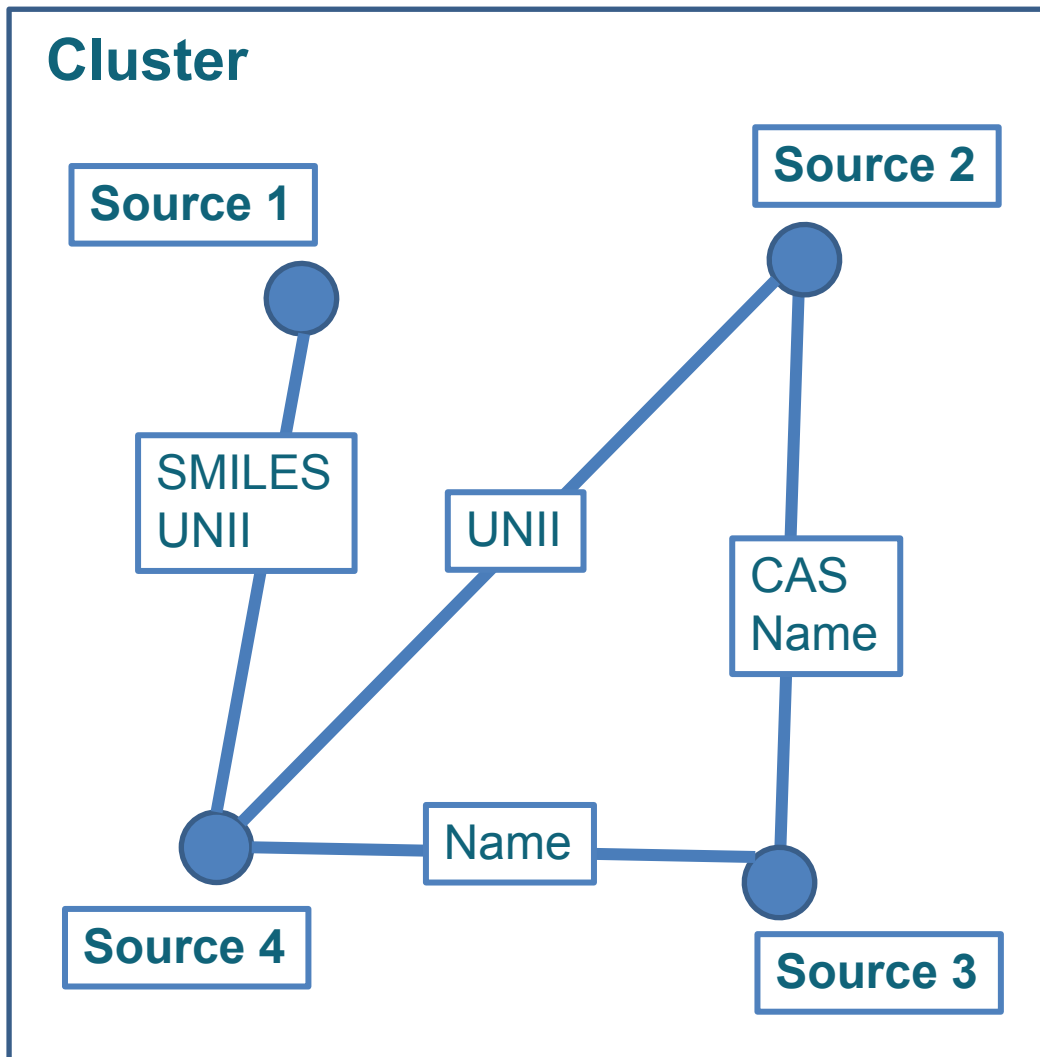
Overview

Inxight Drugs – Comprehensive Collection of Drugs and Substances

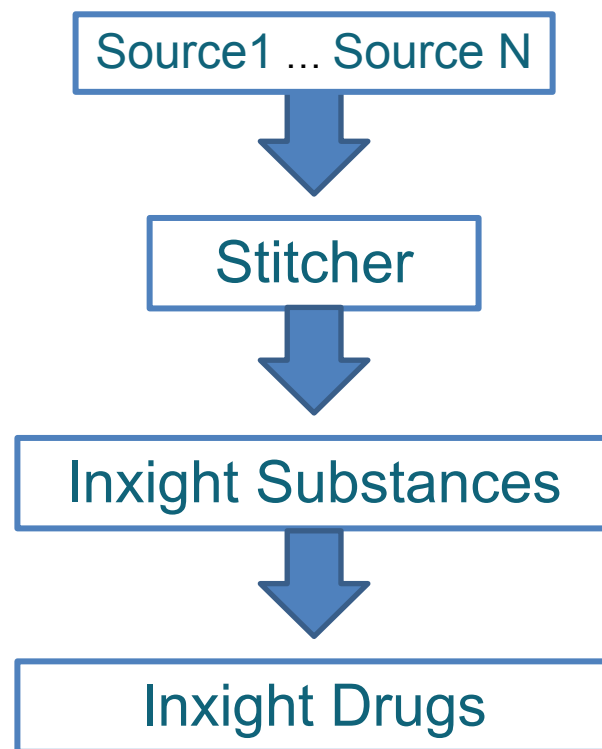
- 5 sources (51 in pipeline)
- 2,741 US Approved Drugs
- 7,298 Entered Clinical Testing
- 99,922 Substances
- 6,684 manually annotated compounds
- Based on NCATS GSRS
- “Stitcher” – NCATS data unification and de-duplication software

NCATS Stitcher


Cluster





- 1 Cluster = 1 Substance
- Canonical Properties
- Parent / Children relationships




NCATS GINAS/GSRS

G-SRS 
version 2.0.01 beta

Browse Substances Structure Search Sequence Search  

Login

▼ Substance Type 

☐ Chemical **63376**


☐ Structurally Diverse **24788**

☐ Concept **5522**

☐ Mixture **2405**

☐ Polymer **2001**

[More ...](#)

▼ Molecular Weight 

☐ 0:200 **27509**

☐ 200:400 **33059**




☐ 400:600 **14106**

☐ 600:800 **3840**

☐ 800:1000 **1413**

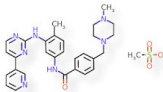
[More ...](#)



99921 << < **1** 2 3 4 5 6 7 8 ... 6245 6246 > >>

Sort By:   


IMATINIB ME

ACHIRAL




- Based on FDA SRS data
- ~90K manually curated records!
- Highly specialized software
- Focus mostly on definitional information
- “Bare-bones” view of data

LYMPHOBLASTIC LEUKEMIA-LYMPHOMA 

IMATINIB MEDAC (AUTHORIZED:

HYPEREOSINOPHILIC SYNDROME)  IMATINIB

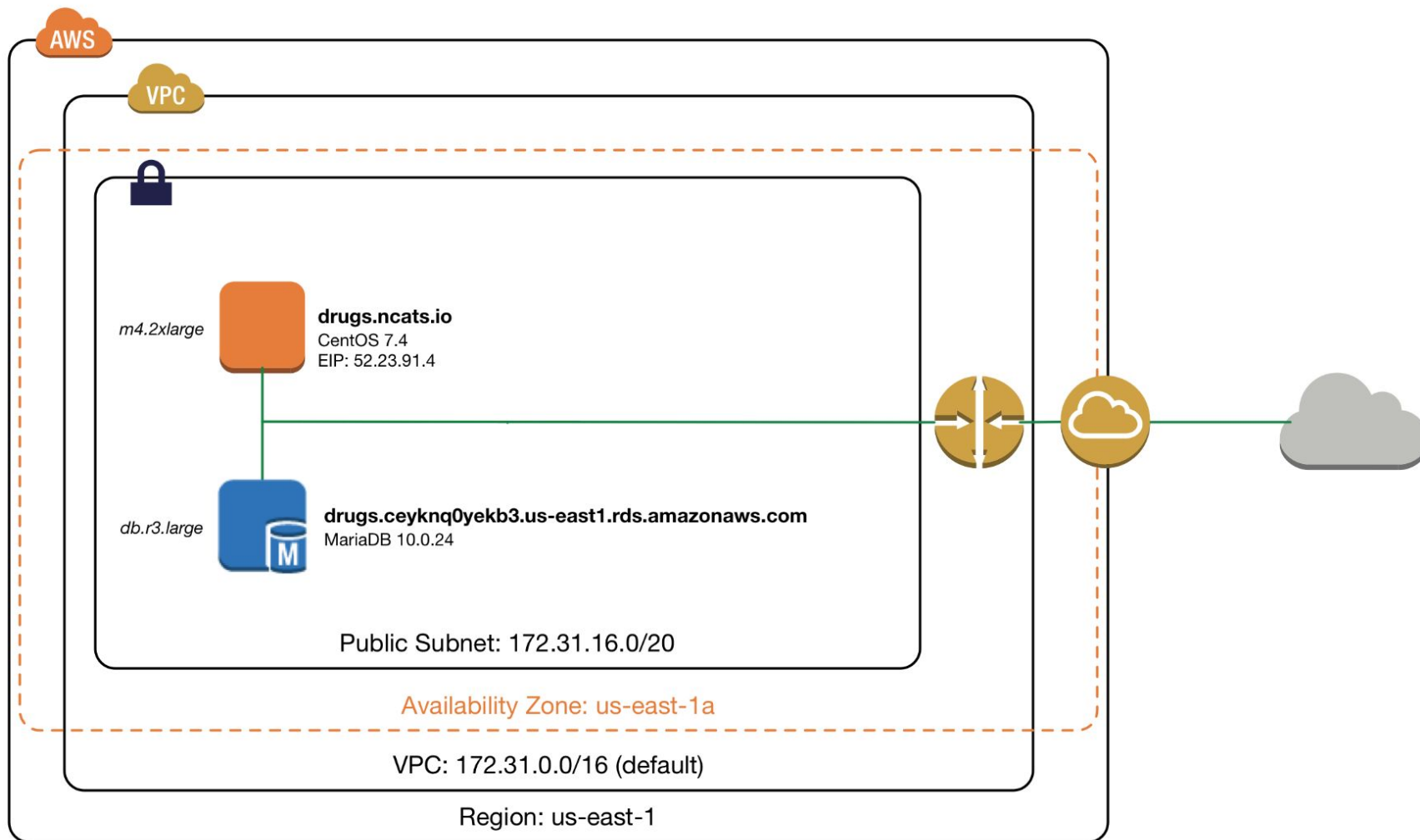
ACTAVIS (AUTHORIZED: LEUKEMIA,

MYELOGENOUS. CHRONIC. BCR-ABL

NCATS Drugs (Production) in AWS

drugs.ncats.io

October 2017



Inxight Drugs

U.S. Department of Health & Human Services National Institutes of Health NCATS



Inxight Drugs



The National Center for Advancing Translational Sciences has developed Inxight Drugs — a comprehensive portal for drug development information.

Inxight incorporates and unifies a wealth of data, including marketing and regulatory status, rigorous drug ingredient definitions, biological activity, clinical use and more.

Inxight incorporates manually curated data provided by the **FDA** and private companies.

Currently, Inxight contains information on:

- 2,741** APPROVED DRUGS
- 3,956** MARKETED DRUGS
- 7,347** ENTERED CLINICAL TESTING
- 99,922** ALL SUBSTANCES

- Intended for wide audience
- Built on ISO 11238 core
- First-in-class data aggregation
- Manually curated data

Drugs List and Filters

U.S. Department of Health & Human Services

National Institutes of Health

NCATS

NIH

National Center
for Advancing
Translational Sciences

Inxight Drugs

▼ Primary Target

☐ DNA 49

☐ Histamine H1 receptor 43

☐ Glucocorticoid receptor 42

☐ Bacterial penicillin-binding protein 38

☐ Dopamine D2 receptor 35

[More ...](#)

▼ Condition

☐ Hypertension 83

☐ Pain 60

☐ Urinary Tract Infections 45

☐ Bacterial Infections 30

☐ HIV Infections 26

[More ...](#)

▼ Approval Year

☐ 1967 213

Number of Drugs by Treatment Modality

Showing 1 - 16 of 2,741 Drugs

<<

<

1

2

3

4

5

6

7

8

...

171

172

>

>>

Sort By

▼

SAFINAMIDE MESYLATE

● ABSOLUTE

Names:

SAFINAMIDE METHANESULFONATE
SAFINAMIDE MESILATE
XADAGO
(S)-2-((4-((3-FLUOROBENZYL)OXY)BENZYL)AMINO)PROP...
NW-1015

Targets:

Monoamine oxidase B 9

glutamate secretion 1

Sodium channel alpha subunit 16

NIH

National Center
for Advancing
Translational Sciences

Drug Record Details

SAFINAMIDE MESYLATE

> Structure

> General

> Activity

> Publications

> Application

> Names 12

> Classification 1

> Identifiers 7

> Related Substances 1

General

Description

Safinamide (FCE 26743, NW 1015, PNU 151774, PNU 151774E, trade name Xadago) combines potent, selective, and reversible inhibition of MAO-B with blockade of voltage-dependent Na⁺ and Ca²⁺ channels and inhibition of glutamate release. Safinamide is under development with Newron, Zambon and Meiji Seika Pharma for the treatment of Parkinson's disease. Safinamide has been launched in the EU, Iceland and Liechtenstein. Safinamide was well tolerated and safe in the clinical development program that demonstrated the amelioration of motor symptoms and OFF phenomena by safinamide when combined with dopamine agonists or levodopa.

CNS Activity

CNS Active 355  

Originator

Farmitalia Carlo Erba (later Pharm...

Approval Year

2017 37


Activity

 Target Info 

 Condition Info 

Primary Target

Sodium channel alpha subunit 16 

glutamate secretion 1 

Monoamine oxidase B 9 

Pharmacology

Blocker 51

Inhibitor 681

Inhibitor 681

Condition

Parkinson Disease

Potency

8.0 μ M [IC50]

56.4 μ M [IC50]

98.0 nM [IC50]

Sources and Definitions

Sources

- 6,684 Compounds manually curated by bioSciences
- 99,393 FDA Substance Registration System
- 14,814 NCATS Pharmaceutical Collection
- 7,039 DrugBank
- 66,870 DailyMed

Definitions

Drug (therapeutic, intervention)

The "platonic", idealized form of an active pharmaceutical ingredient included in or produced by a currently or previously marketed drug product to contribute to the pharmacological action used to treat a condition. Usually an active moiety, except for prodrugs.

DEMO

Summary

- **Content and Purpose**

Complete drug development profile:
from structural details to drug products.

- **Core Components**

Precise scientific definition for the all the ingredients in medical products, as per the rigorous ISO 11238 definition.

- **Data Quality**

Enormous amount of manually curated data: 90K entries from FDA SRS and 7K annotations from Rancho BioSciences

- **Data Aggregation**

First-in-class automated facile data aggregation from multiple sources via Stitcher (5 implemented, 51 in the pipeline)

<https://drugs.ncats.io>