

GSRS & Inxight Drugs

An Introduction to NCATS Public Resources and Analytics for Rare Diseases, Targets, Drug Substances, and Analytes

Session Number: W20

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Defining standards for medicinal products

Global Substance Registration System – developed by NCATS DPI Informaticians

Registration and Public Access to
Data on substances found in
medicinal products

- First ISO 11238 Standard Compliant Substance Registration System
- Broad adoption: FDA, WHO, European Medicines Agency, United States Pharmacopeia, etc
- Includes small molecules, antibodies, gene and cell therapies, antisense oligos, etc

The screenshot shows the GSRS website interface. The header includes the GSRS logo (Ver. 3.0.3), a menu icon, a search bar labeled 'Search Substances', and a login link. The left sidebar contains 'Quick Links' for 'Substances' (with a link to 'Browse Substances') and 'Register' (with links for 'Chemical' and 'Protein'). The main content area features a banner with four images (pills, chemical structures, DNA, and a molecular model) and the title 'Global Substance Registration System - GSRS'. Below this is a search bar and four buttons: 'Browse Substances', 'Structure Search', 'Sequence Search', and 'Bulk Search'. A table displays the total number of substances (145,291) and a breakdown by category:

Total substances: 145,291				
Chemicals	100,360	Polymers	2,396	Structurally Diverse
Proteins	6,417	Nucleic Acids	438	Concepts

<https://gsrs.ncats.nih.gov>

Collaboration with the FDA

Augmenting Information on Medicinal Products

Information on marketing and regulatory status, ingredient definitions, biological activity, clinical use, and more

Public, curated data from the FDA, NCATS, and private companies

US APPROVED DRUGS: **2,620**

MARKETED DRUGS: **11,847**

INVESTIGATIONAL DRUGS: **9,748**

ALL SUBSTANCES: **144,045**

drugs.ncats.io/

Siramshetty et al, NAR 2022

Tools for navigating data in GSRS and Inxight

Text search

Structure Search

Sequence Search

Downloads

- GSRS download
 - <https://gsrs.ncats.nih.gov/#/release>
- Inxight partial download
 - <https://drugs.ncats.io/downloads-public>

Find a drug

Structure search

Sequence search

- FVNQHLCGSHLVEALYLVCGERGFFYTKPT

Downloads

Programmatic access to Inxight Drugs

API: <https://drugs.ncats.io/api/v1>

Search

- <https://drugs-02.ncats.io/api/v1/substances/search?top=25&skip=0&q={{term}}>

Details

- [https://drugs.ncats.io/api/v1/substances\({{UUID or UNII}}\)?view=full](https://drugs.ncats.io/api/v1/substances({{UUID or UNII}})?view=full)

Additional Details

- [https://drugs.ncats.io/api/v1/substances\({{UUID or UNII}}\)/@additional?view=full](https://drugs.ncats.io/api/v1/substances({{UUID or UNII}})/@additional?view=full)

Programmatic access to GSRS

GSRS data is available via download

- <https://gsrs.ncats.nih.gov/#/release>

KNIME workflow to help you start digging in to that download

- <https://hub.knime.com/> search for “GSRS”

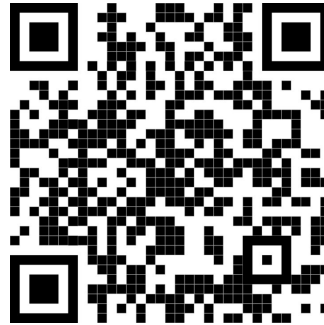
Let's make this interactive

***All workshop materials
can be found here:***



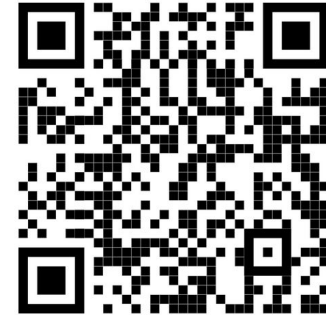
<https://shorturl.at/kvzIZ>

***Some installation
prerequisites for
RaMP-DB:***



<https://shorturl.at/bgqrQ>

***Provide your
comments/thoughts
here:***



<https://shorturl.at/sS138>

Thank you!

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