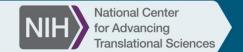
GSRS Development Update

30 October 2019

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DANNY KATZEL
FDA
NIH/NCATS





Agenda

High Level GSRS Core Status

- 2.4 Release
- spotlite migration
- G-SRS 3.0 technology upgrade
- Resource Updates



GSRS Release Status

- GSRS FDA Production Releases
 - 2.3.7 June 2019
- Upcoming GSRS FDA Releases
 - 2.4 scheduled for late Oct 2019
 - 3.0 development Spring 2020



GSRS 2.4 Release Update

Updates available in the 2.4 public release

- Substructure Search now includes Polymers
- Calls to underlying chemical library have been refactored to allow for future swapping out at runtime.
- Structure Rendering improvements including bracket and S group support
- new Angular BETA UI
- Migrated Bookmarklets and other Powertools to UI
- Bug fixes, additional validation rules
- API improvements
 - URLs now have full UUIDs instead of just first 8 chars
 - ID resolvers for other names



Advanced Functions in Edit Mode

Advanced functions *

Standardize names

Reset definitional References

Set definition to private

Set definition to public

Restore SRU amounts from previous version

Change substance class

Set status to pending

Set status to approved

Merge and deprecate subconcept record

Un-approve record (Remove approval ID)

Change approval ID

Add a fragment to CV

Switch primary with alternative definition



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GIT Code Repository Migration to GitHub

The Current GIT repository server https://spotlite.nih.gov/ncats/inxight is being decommissioned by NCATS.

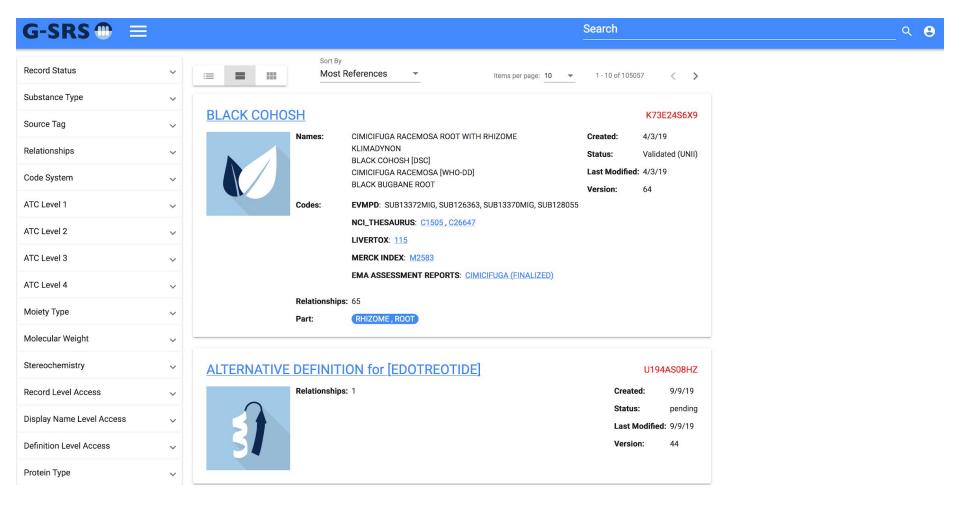
We will move to github in November 2020

spotlite server will stay up in read only mode for a brief period to allow for smoother transition.

We will send out instructions for how to repoint local repositories in November



Beta UI





GSRS 3.0 Technology Upgrade

Backend Upgraded to latest Industry Standards

	2.x	3.0
Java version	7/8	11
Framework	Play 2.3	Spring-boot 2.2
ORM	Ebean	Hibernate
dependency management	manual global state	dependency injection



Resource Updates

- Update to the Swagger Documentation
- User Guide
- Data Dictionary
- JSON Schema



User Guide for Registration

Metabolite relationships always link to active moiety/prodrug. The relationship options between metabolites and the active moiety/prodrug are:

- Active
- Active → (as) Parent
- Active → Prodrug
- Inactive → Parent
- Less Active → Parent
- → Parent (unknown)
- Toxic → Parent (without any activation)
- Reactive Type → Parent
 - o Those should be covalently bind to proteins and nucleic acids for the toxicity

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2952084/

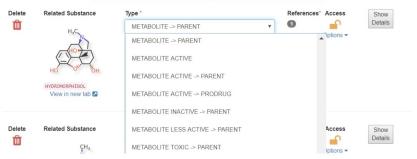


Figure 31 - Register Chemical - Relationships - Metabolite Types

Example: Noroxymorphone is an active metabolite of oxycodone.

- Edit Oxycodone
- 2. In the Relationships card, click Add another relationship
- 3. In Related Substance, search and select "Noroxymorphone"
- 4. For Type, select "METABOLITE ACTIVE -> PARENT"
- Add a Reference a reference is required. If references already exist, you can select an existing reference or Add a Reference





https://tripod.nih.gov/ginas/#/release



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Release Notes

G-SRS v2.3.3 (February 25, 2019)

Download with data



Download software only



Download sample data



Disclaimer:

The data provided is test data from an incomplete migration of public data from the FDA and other sources. While efforts are made to continually improve the quality of the data presented in the seed data set, it is neither complete nor validated at this time. It serves as example data only. If you spot an error, please let us know.

Other Downloads

- Gings Excel Tools
- Full Public Data Dump
- GSRS Data Dictionary
- GSRS JSON schema

Quick Links

- System Requirements
- Installation Instructions
- Database Connection
- User Registration
- Data Loading
- Questions



ANIOFICO

Thank you

Collaborator Slack channel (ask us to add you)

https://gsrscollaborator.slack.com

