GSRS Development Update

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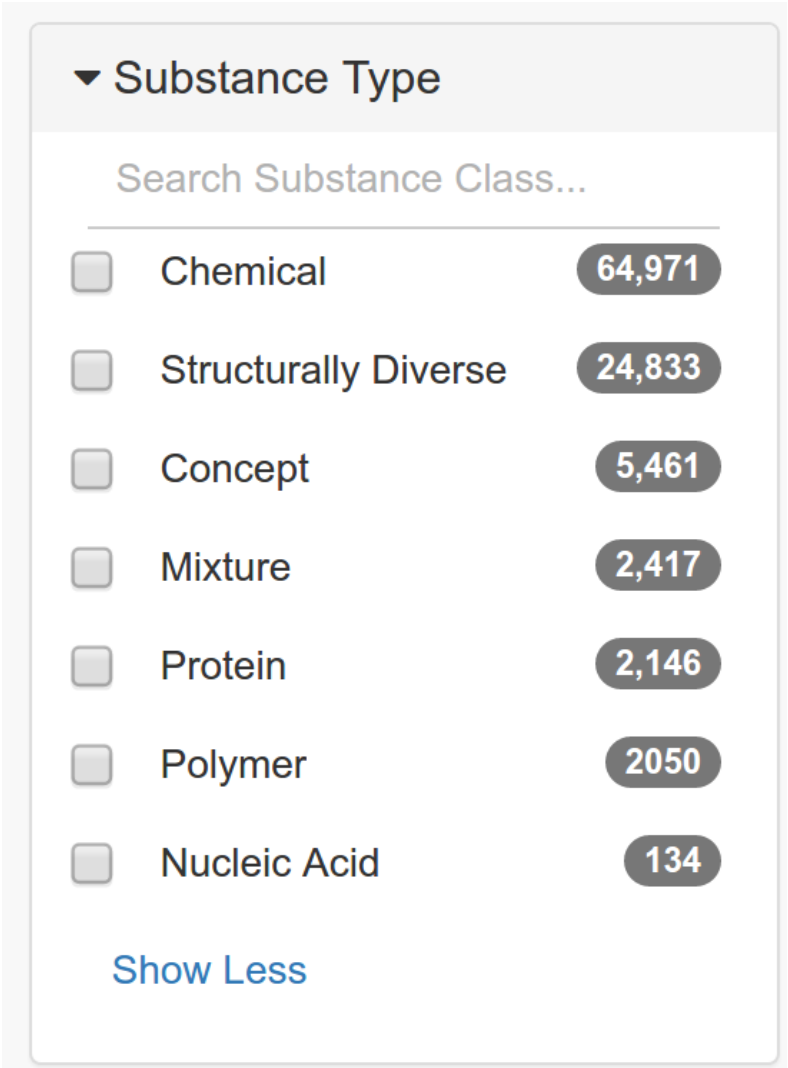
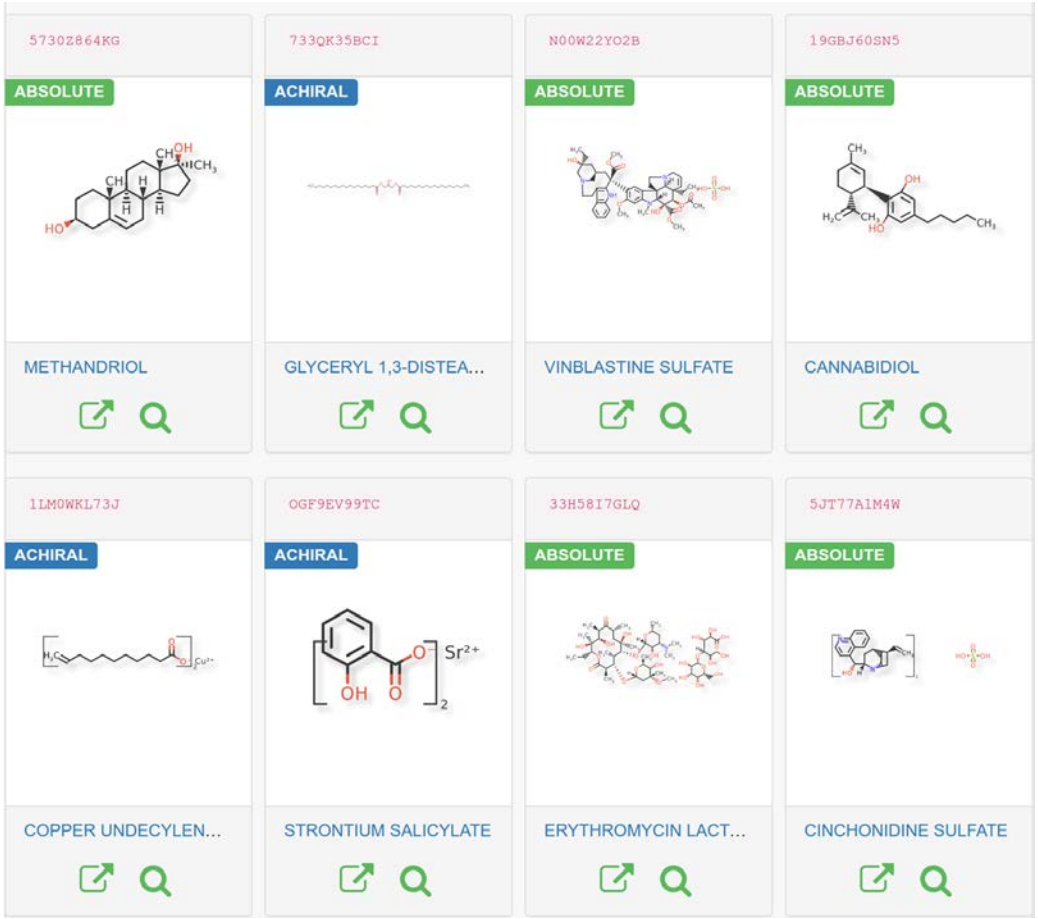
GSRS Status

High Level GSRS Core Status

- GSRS 2.3.1 in production at FDA (October 2018)
  - 2.3.1 public released
- GSRS 2.3.2 development (November 2018)
  - Pre-production at FDA
  - Pending public release soon (December 2018)
- GSRS 2.4 development (1st quarter 2019)
  - In development
  - Improved data exchange / communication

GSRS Status





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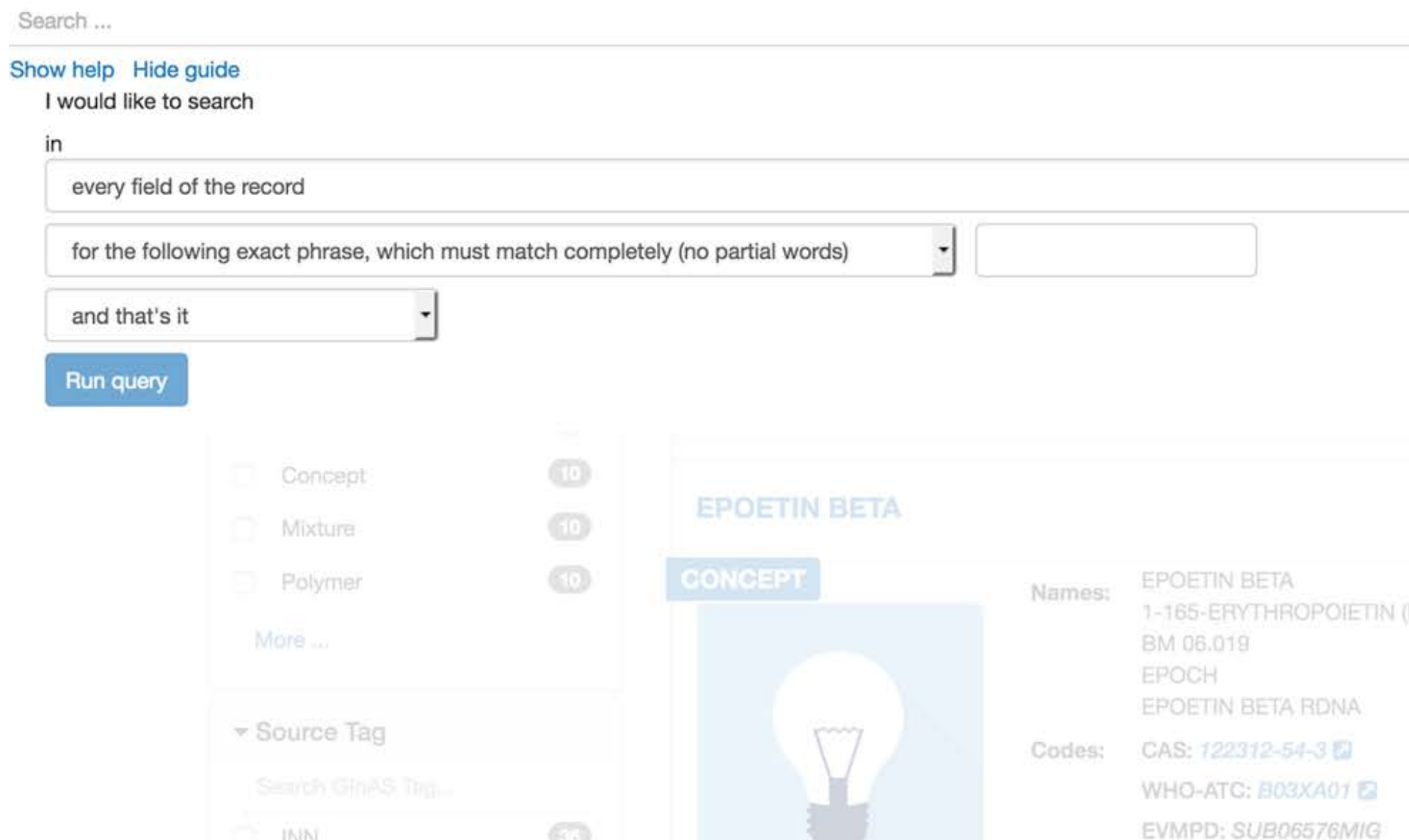
GSRS 2.3.1 Status

- **GSRS 2.3.1 Improvements**
  - Substance “Hierarchy” views
  - Additional Validation Rules
  - Improved Relationship Handling
  - Improved Structure Resolver
  - Configurable / modular Validation Engine
  - Porting of some FDA-specific enhancements to main code base
  - Bug fixes
  - Improved UI
  - New Guided Search

GSRS 2.3.1 New Search Guide



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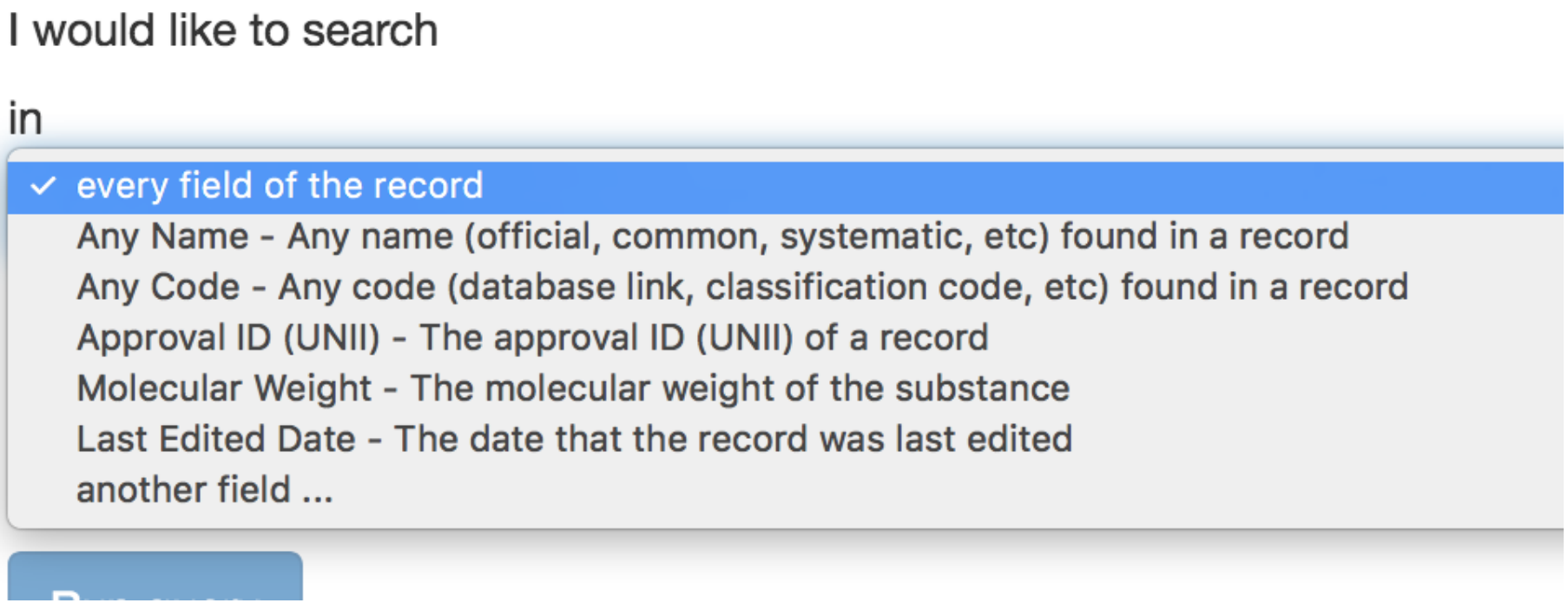

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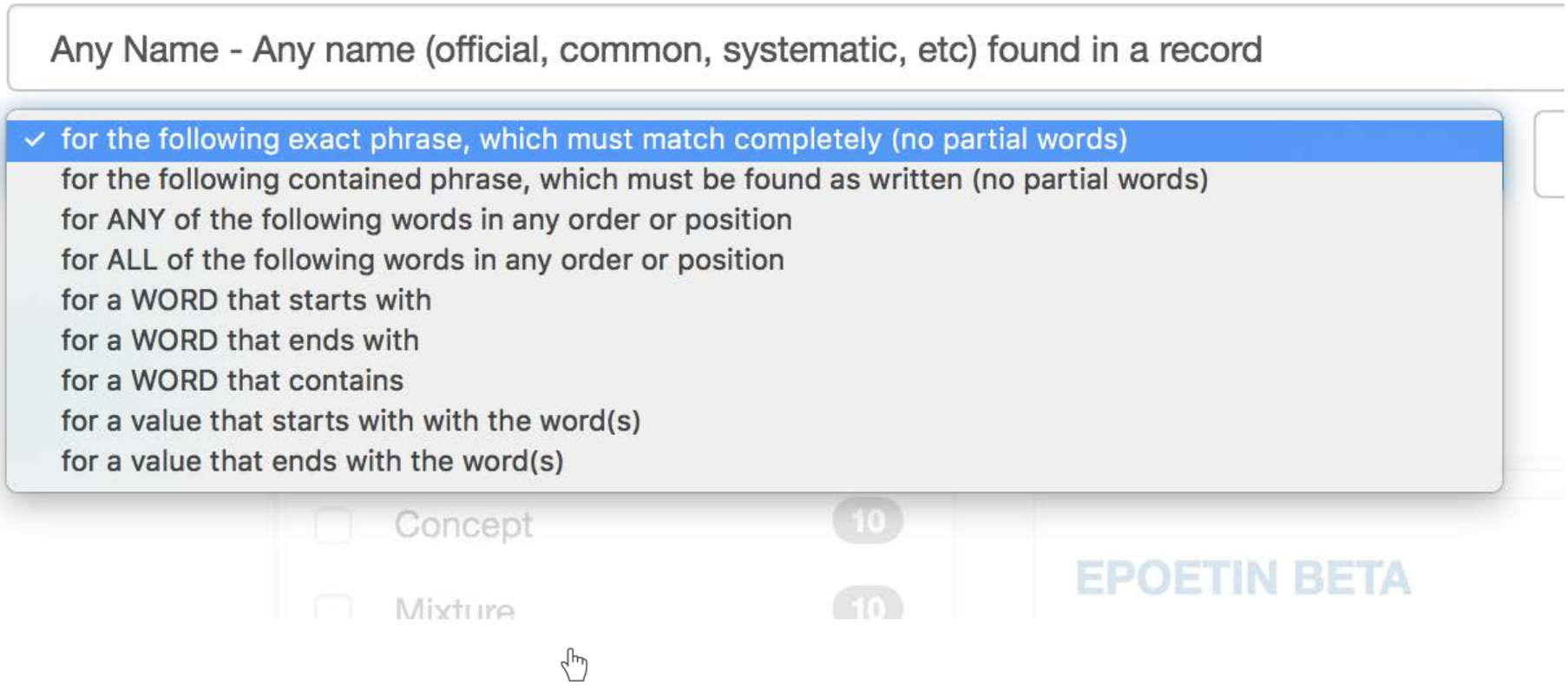

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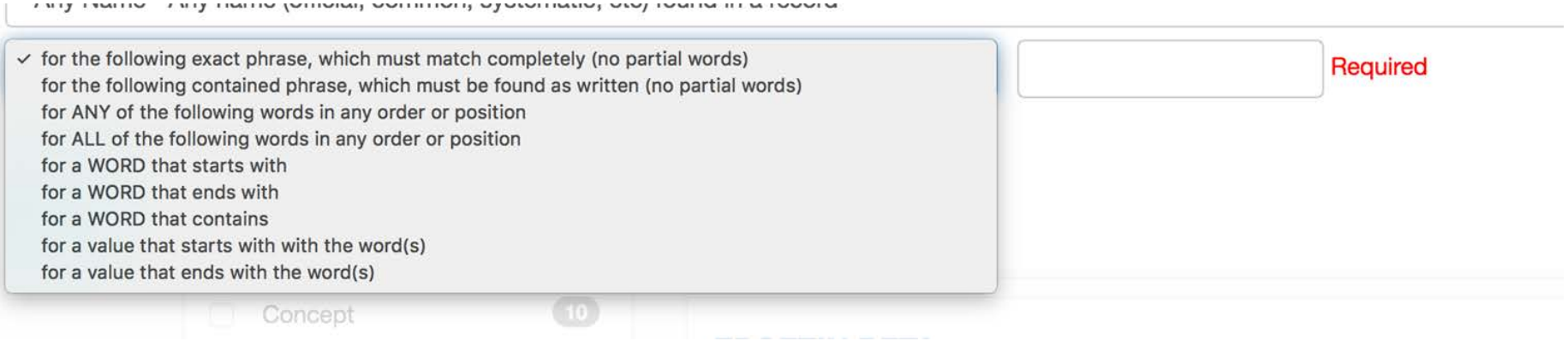

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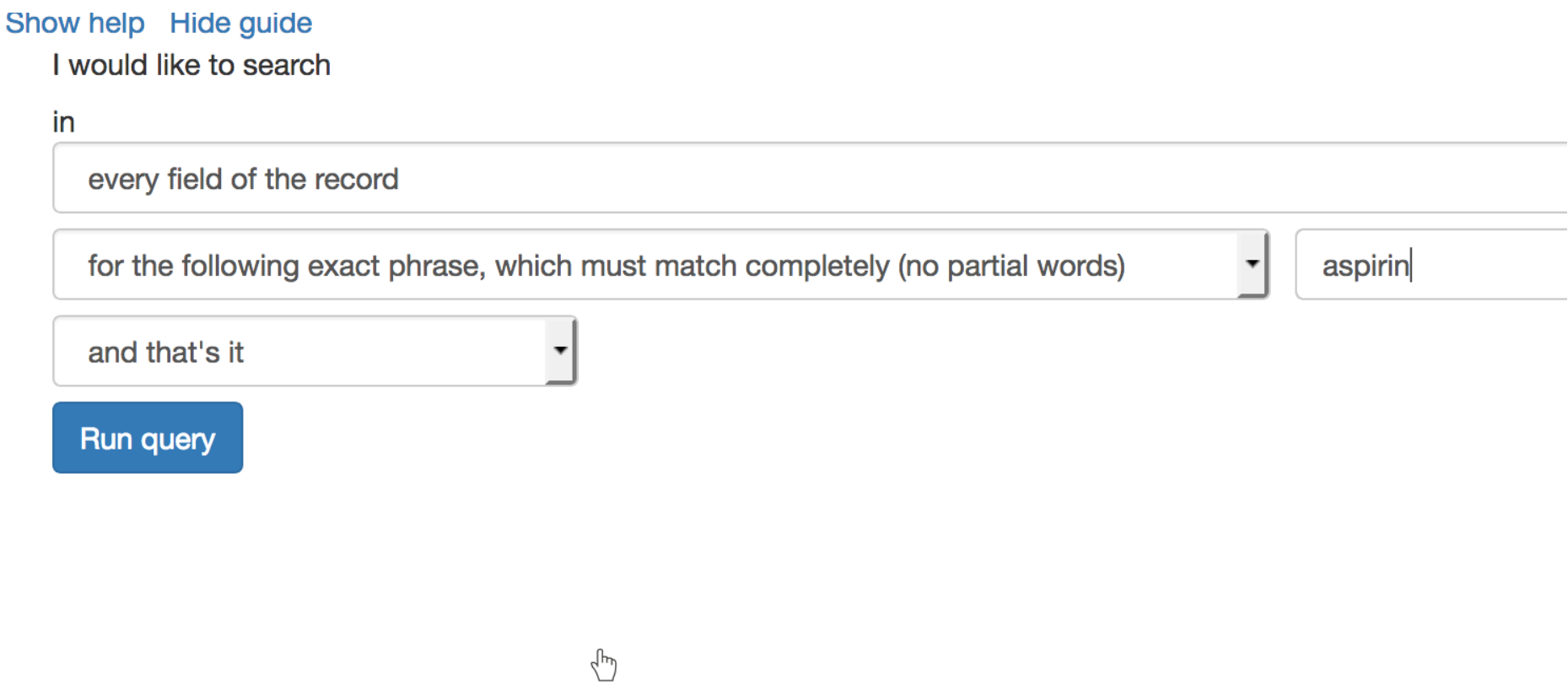

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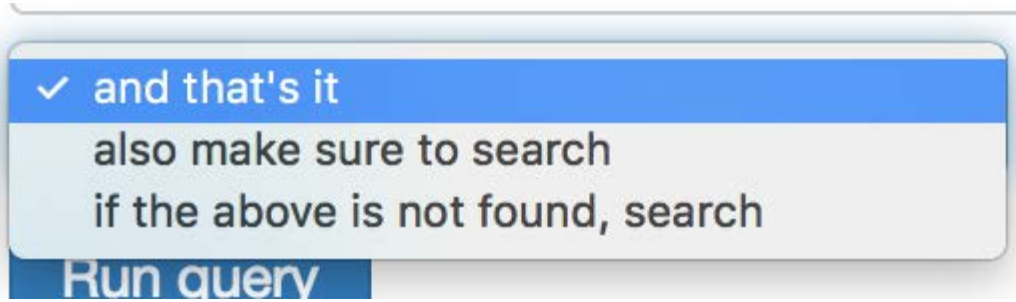
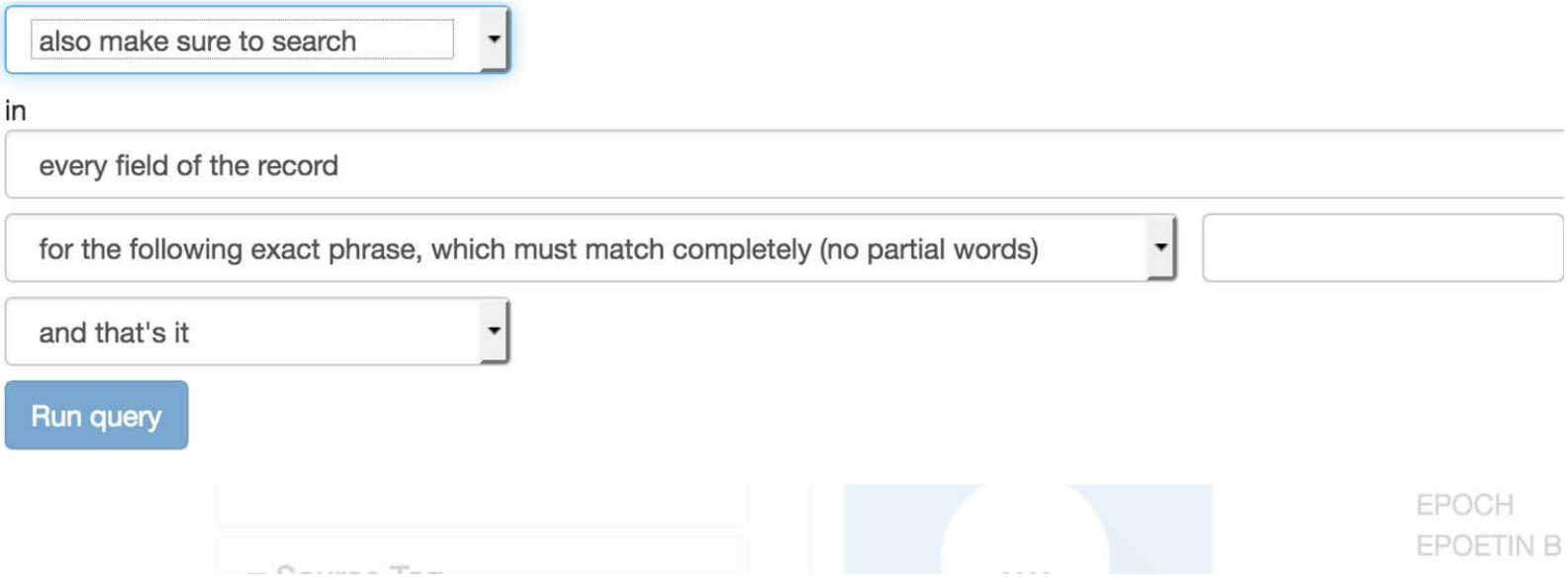




GSRS 2.3.1 New Search Guide

root_names_name:"^aspirin$" OR "^foo$"

Show help Hide guide

I would like to search

in

Any Name - Any name (official, common, systematic, etc) found in a record

for the following exact phrase, which must match completely (no partial words) | aspirin

if the above is not found, search

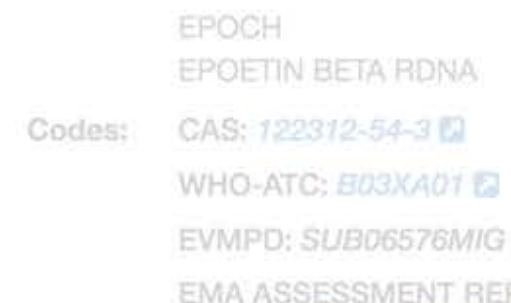
in

every field of the record

for the following exact phrase, which must match completely (no partial words) | foo

and that's it

Run query

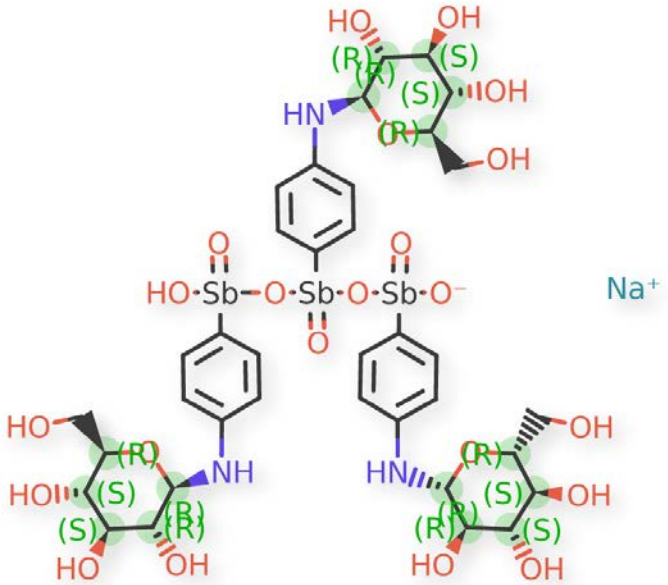


GSRS 2.3.2 Status

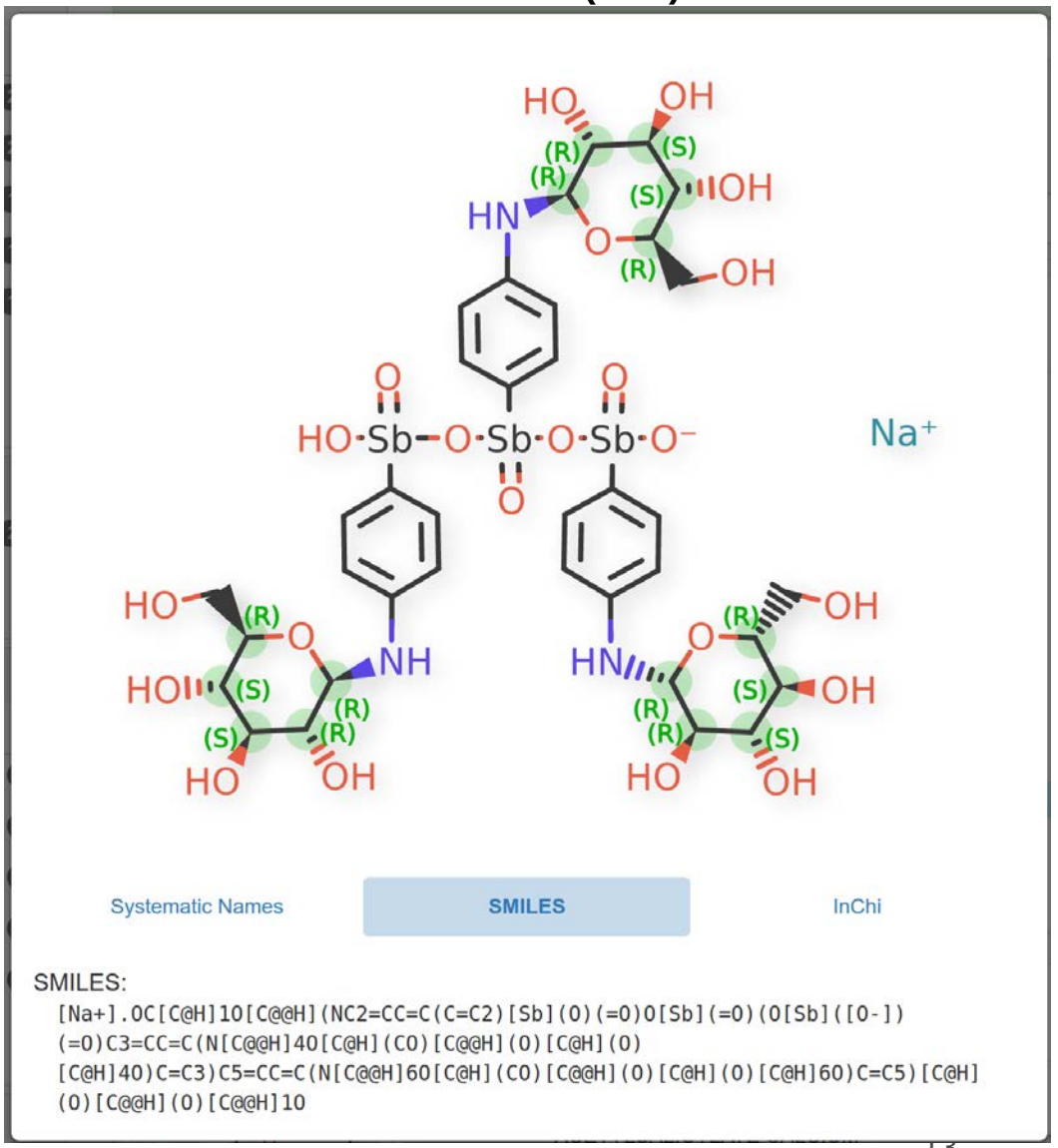
- **GSRS 2.3.2 Improvements**
  - Improvements to rendering of molecules
  - Further improvements to guided search
  - Further improvements to duplicate check / sequence searching
  - Ability to easily revert records for authorized users
  - Additional stability and data integrity checks
  - Improvements to hierarchy view

GSRS 2.3.2: Rendering

GSRS 2.3.1 (old)



GSRS 2.3.2 (new)



GSRS 2.3.2: Guided Searches

GSRS 2.3.1 (old)

(a little opaque and inaccurate)

Searched for:
root_structure_mwt *: [100 TO 10E50] AND aspirin (contains)*

GSRS 2.3.2 (new)

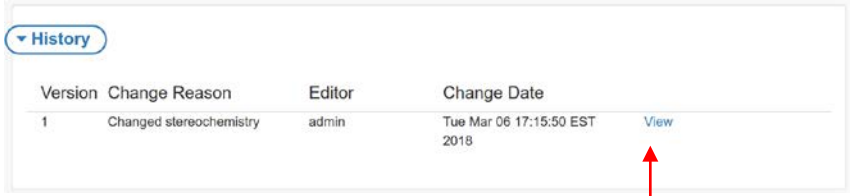
(more informative and accurate)

You searched *for the* ***Molecular Weight*** *field >* ***100*** *AND for any field = ...****aspirin****...* *show long explanation*

You searched *in the* ***Molecular Weight*** *field, for a value or values that must greater than* ***100****. Also making sure to search in any field, for a value or values that contains* ***aspirin*** *show short explanation*

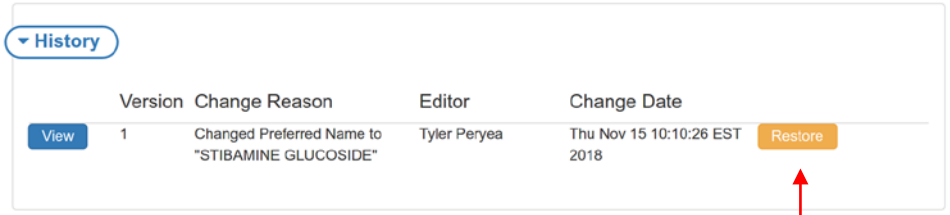
GSRS 2.3.2: Restoring Old Versions

GSRS 2.3.1 (old)



Super users can **view** old versions, but involved process to revert

GSRS 2.3.2 (new)



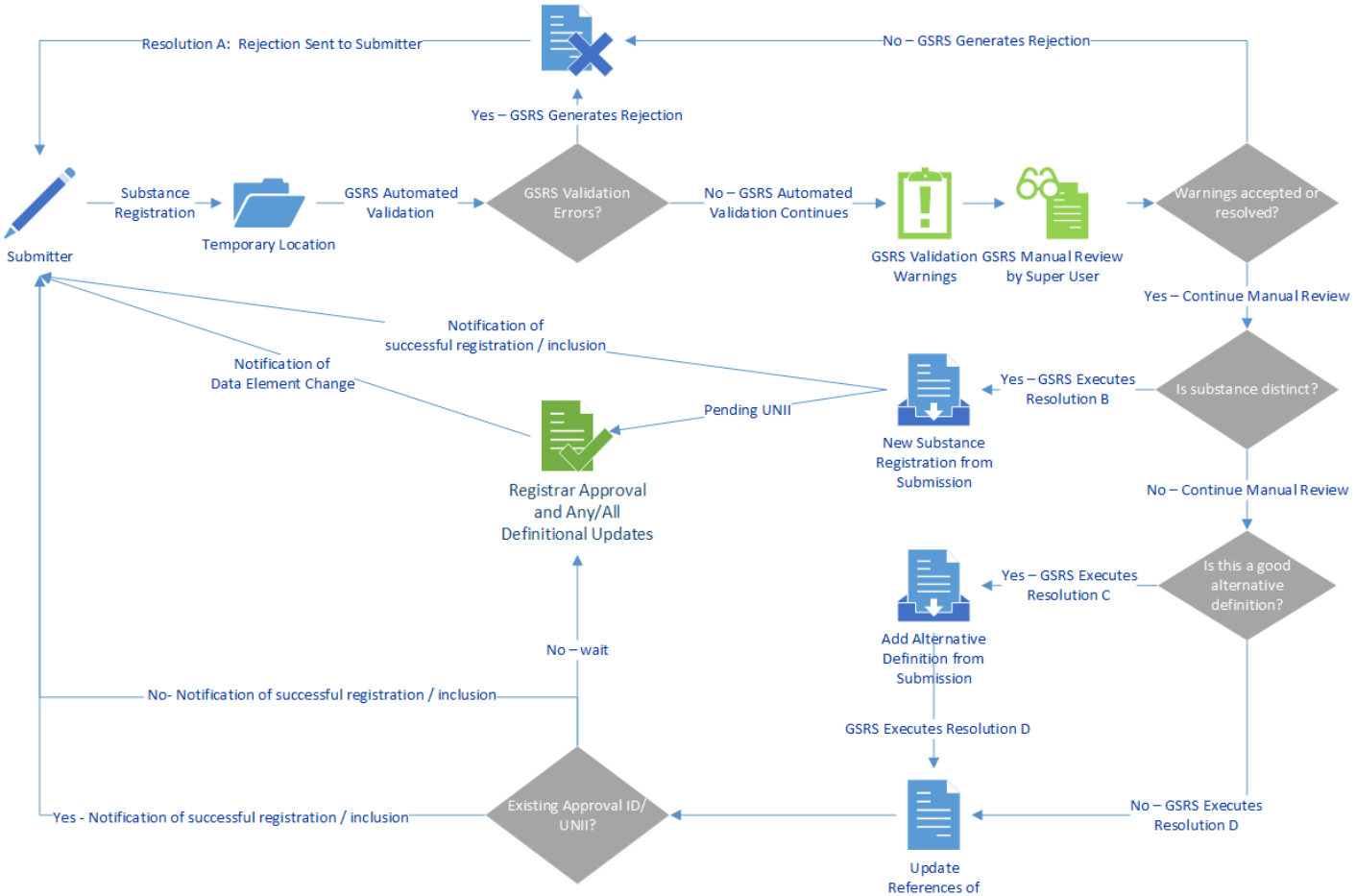
Super users can quickly **revert** records, after review

GSRS Status

On the horizon

- GSRS 2.4
  - Submissions / System-to-system communication
    - Establishment of requirements document *(complete)*
    - Basic support for accepting / staging / processing new and modified records from external sources *(1st quarter 2019)*
  - Simplified installation / launch
    - High-level feasibility report *(complete)*
    - Basic support *(1st quarter 2019)*

System Submission and Exchange Mechanism



- Green indicates existing functions/processes
- Blue indicates update required to GSRS (primarily to automate, manual processes already supported)

GSRS Status

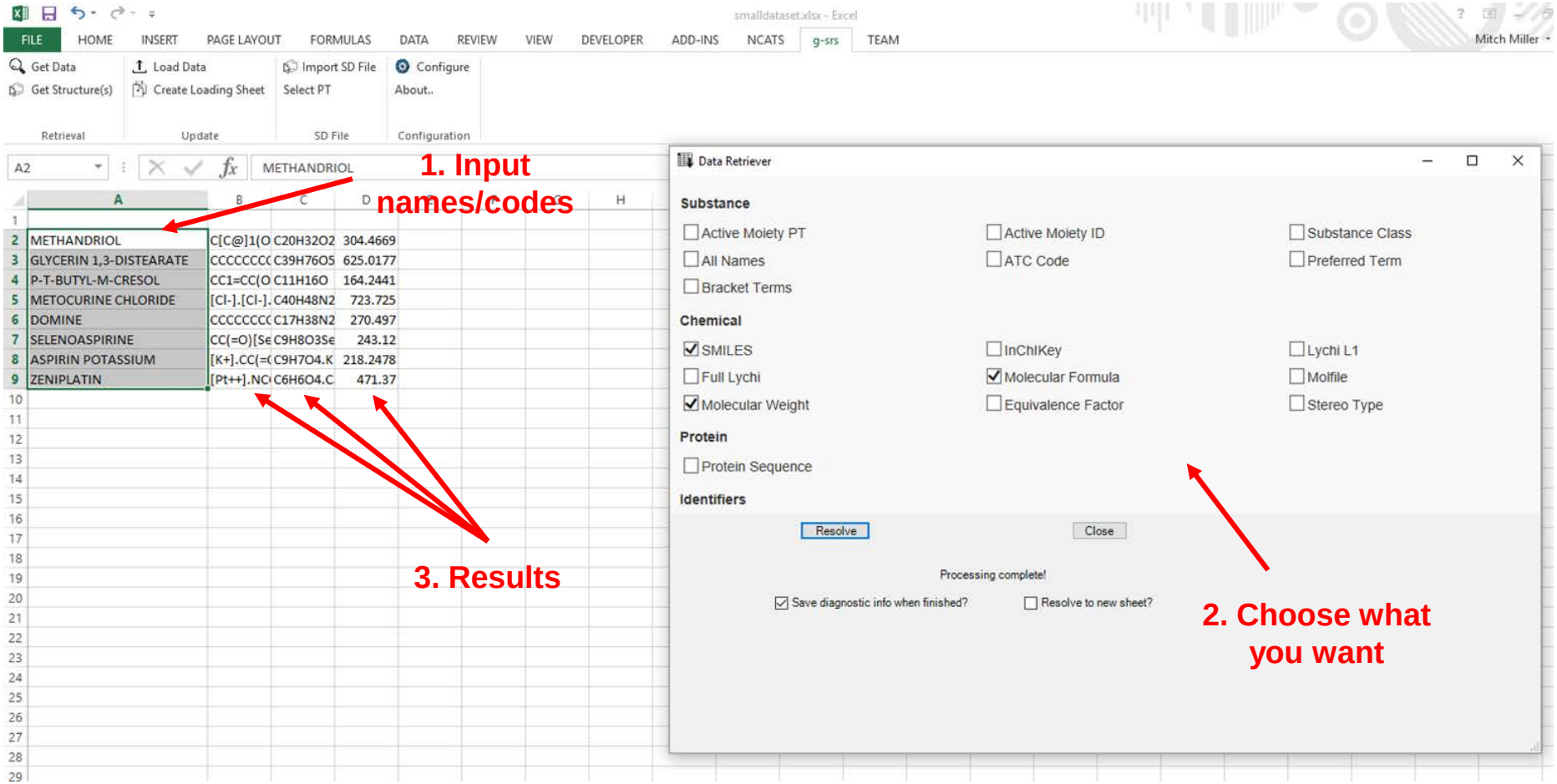
On the horizon

- GSRS 2.5+
  - Improvements to REST API / Systematic access
  - Upgrade of UI to modern web framework for client-side UI
    - Angular 6+
    - Websocket support

GSRS Tools

- **GSRS Find excel tool** *(currently in alpha release)*
  - Search, create, update, retrieve records and substance information in batches
  - Support for loading SD files
- **Stand-alone Java API library** *(1st quarter 2019)*
  - Easier programmatic access to data for integration with other applications / stand-alone tools
- **Stand-alone Javascript API library** (2nd quarter 2019)
  - Provides simple communication and data operations with running instance

GSRS Tools: GSRS Find



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

GSRS Tools: Stand-alone Java API Library

```
try(GsrsRestClient client = DefaultGsrsRestClient.create("https://ginas.ncats.nih.gov/ginas/app")){

        GsrsSearchResult result = client.searcher().substructure("C1=CC2=CC=CC=C2C=C1");

                System.out.println("search results :");
                System.out.println("total : " + result.getTotal());
                System.out.println("top 10 substance names:");

                result.getUuids()
            .stream()
                        .limit(10)
                        .forEach(uuid->{
            try {
                Substance sub = client.fetchSubstance(uuid);

                System.out.println(sub.getName());
            }catch(IOException e) {}});


}
```

```
search results :
total : 1973
top 10 substance names:
NAPHTHALENE
POLYCYCLIC AROMATIC
HYDROCARBONS
PHENANTHRENE
ANTHRACENE
BENZ(A)ANTHRACENE
TRIPHENYLENE
CHRYSENE
BENZO(C)PHENANTHRENE
TETRACENE
DIBENZ(A,H)ANTHRACENE
```

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

Acknowledgements

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Questions