# GSRS Development Update

27 June 2018

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**NIH/NCATS**

NCATS

National Center
for Advancing
Translational Sciences

# GSRS Status

## High level GSRS Core status

- GSRS 2.2 in production at FDA

- Public release of 2.2 by mid July

- GSRS 2.3 development

  - Porting certain FDA-enhancements to core code

  - Improving modularity

  - Additional features

# GSRS Status

- **GSRS 2.2 Improvements**
  - Bug fixes
  - Improved Modular UI for record views
    - "Cards" UI
  - Additional Validation Rules
  - Additional Configuration Options
    - Sequence Search Configuration Options
    - Cache Configuration Options
    - UI Configuration Options
    - Admin-level Configuration Options
  - Improved Relationship Handling
  - Improved Structure Resolver

# GSRS 2.2 Status: Cards

**ARGIPRESSIN**

Y490706MFD

> Overview

> Names — 15

> **Classification** — 2

> Identifiers — 6

> Subunits — 1

> Disulfide Links — 1

> Active Moiety — 1

> Modifications — 1

> Characteristic Attributes — 1

> Notes — 1

> Audit Info

> References — 25

▼ Classification

Show 5 entries                                                    Search ...

| Classification Tree | Code System | Code |
| --- | --- | --- |
| ATC<br>SYSTEMIC HORMONAL PREPARATIONS, EXCL. SEX HORMONES AND INSULINS<br>PITUITARY AND HYPOTHALAMIC HORMONES AND ANALOGUES<br>POSTERIOR PITUITARY LOBE HORMONES<br>Vasopressin and analogues<br>argipressin | ⓘ WHO-ATC | H01BA06 |
| VATC<br>PITUITARY AND HYPOTHALAMIC HORMONES AND ANALOGUES<br>POSTERIOR PITUITARY LOBE HORMONES<br>Vasopressin and analogues<br>argipressin | ⓘ WHO-VATC | QH01BA06 |

Showing 1 to 2 of 2 entries                          Previous  **1**  Next

▼ Identifiers

Show 5 entries                                                    Search ...

| Code System | | Code | Type | Description |
| --- | --- | --- | --- | --- |
| CAS | ⓘ | 113-79-1 | PRIMARY | |
| NCI_THESAURUS | ⓘ | C926 | PRIMARY | |
| MESH | ⓘ | D001127 | PRIMARY | |

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# GSRS 2.2 Status: Cards



```
cardView.substanceDetails = [
...
        {
                substanceClass : "ix.ginas.models.v1.Substance",
                cardClass : "ix.ginas.utils.views.cards.ClassificationsCard"
        },
...
        {
                substanceClass : "ix.ginas.models.v1.ProteinSubstance",
                cardClass : "ix.ginas.utils.views.cards.SubunitsCard"
        },
        {
                substanceClass : "ix.ginas.models.v1.ProteinSubstance",
                cardClass : "ix.ginas.utils.views.cards.DisulfidesCard",
                viewType : "Substance"
        }
```

# GSRS 2.2 Status: Cards

**ARGIPRESSIN**

Y490706MFD

> Overview
> Names                    15
> **Classification**        2
> Identifiers               6
> Subunits                  1
> Disulfide Links           1
> Active Moiety             1
> Modifications             1
> Characteristic Attributes 1
> Notes                     1
> Audit Info
> References               25

**▼ Classification**

Show 5 ▼ entries

| Classification Tree |
|---|
| ATC |
| SYSTEMIC HORMO |
| PITUITARY AND |
| POSTERIOR |
| Vasopres |
| argip |
| VATC |
| PITUITARY AND HY |
| POSTERIOR PIT |
| Vasopressin |
| argipress |

Showing 1 to 2 of 2 entrie

**▼ Identifiers**

Show 5 ▼ entries

| Code System |
|---|
| CAS |
| NCI_THESAURUS |
| MESH |

```
cardView.substanceDetails = [
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                cardClass : "ix.ginas.utils.views.cards.SubunitsCard"
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        }
```

# GSRS 2.2 Status: Cards

- **Cards UI Advantages**
  - Configurable via configuration file
    - No code changes / recompiling is required to adapt basic UI elements
  - Extendable
    - FDA has ported their custom UI elements to this framework
    - Other customizations possible by implementing a specific Java Interface
  - Modular
    - Extensions can now be separated from the main code base
  - More Consistent
    - Previous ad-hoc customized UI elements often fell out-of-sync with major style changes

# GSRS 2.2 OS Support: Windows

- Windows OS to no longer be officially supported for *production* deployments of GSRS
  - Justification:
    - *Play! Framework* does not officially support Windows deployments
    - The majority of configuration issues for external users of GSRS result from attempts to use Windows deployments
    - Workarounds exist for lack of direct Play! support, but are brittle
    - Build and execution helper scripts are challenging to maintain for both Windows and UNIX environments.
    - Every known production instance of GSRS is currently run from a UNIX-based environment
  - Notes:
    - Using Windows for *development* and *testing* is still supported.
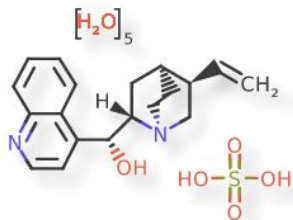    - A Windows *deployment* version may be available again in a different form.

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# GSRS 2.3 Status

## High level GSRS Core status

- GSRS 2.3 developments
    - Configurable / modular Validation Engine
    - Substance "Hierarchy" views
    - Porting of some FDA-specific enhancements to main code base

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# GSRS 2.3 Preview: Hierarchy

**ABSOLUTE**



**Names:** CINCHONIDINE, SULFATE (1:1), PENTAHYDRA...
CINCHONIDINE SULFATE PENTAHYDRATE
CINCHONAN-9-OL, (8.ALPHA.,9R)-, SULFATE (...

**Codes:** CAS: *5907-43-7* ↗

PUBCHEM: *71586828* ↗

**Relationships:** 1

**Formula:** C19H22N2O.5H2O.H2O4S

**Mol Weight:** 482.55

◢ 🔍 CINCHONIDINE [1U622LRA8Z]

    🔍 CINCHONIDINE DIHYDROCHLORIDE [QNY56C6XYZ]

    🔍 CINCHONIDINE HYDROCHLORIDE [694B15YWQK]
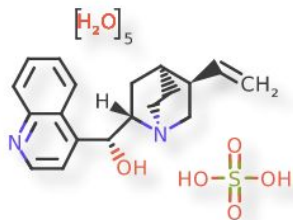
    🔍 CINCHONIDINE [1U622LRA8Z]

    🔍 CINCHONIDINE SALICYLATE [Q1Y52JQ86J]

    🔍 **CINCHONIDINE SULFATE PENTAHYDRATE [P424MD870D]**

    🔍 CINCHONIDINE HYDROCHLORIDE DIHYDRATE [01TO0B37BE]
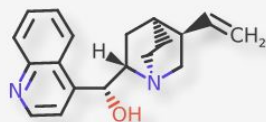
# GSRS 2.3 Preview: Hierarchy



**ABSOLUTE**

$[H_2O]_5$

## CINCHONIDINE SULFATE …

**ABSOLUTE**

CINCHONIDINE

**Names:** CINCHONIDINE, SULFATE (1:1), PENTAHY...
CINCHONIDINE SULFATE PENTAHYDRAT...
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   🔍 CINCHONIDIN
   🔍 CINCHONIDIN
   🔍 CINCHONIDIN
   🔍 **CINCHONIDIN**
   🔍 CINCHONIDIN

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# GSRS Status

## On the horizon

- GSRS 2.2 Public Release (July 2018)
  - New Public Data (July 2018)
- GSRS 2.2.1 FDA production roll-out (July 2018)
  - Maintenance Release
- GSRS 2.3 FDA production roll-out (August 2018)

- System-to-system communication pipeline (2018)
- Bug fixes (continual)
- Improved support for additional substance information (2018)