

INSTALLING THE GINAS, PUBLIC VERSION ON UBUNTU 16.04  
USING POSTGRESQL 10 AS DATABASE

Ginas Monthly Meeting  
Feb 7th, 2017  
Alex Welsch

- A. Slides
- B. Details with CLI commands below

# A.Slides

## Get the program and sample data

<https://tripod.nih.gov/ginas/#/gsrs/>

The screenshot shows a web browser window with multiple tabs. The active tab is titled 'G-SRS Software' and displays the 'Starting with G-SRS' page. The page features a dark blue header with the 'ginas' logo and navigation links for 'Getting Started', 'Documentation', and 'FAQ'. Below the header, the main content area has a dark blue background with the text 'Starting with G-SRS' and 'Download and installation instructions'. A red box highlights the version 'G-SRS v2.0 (October 12, 2017)'. Underneath, there are three download options: 'Download with data' (with a document icon), 'Download software only' (with a download icon), and 'Download sample data' (with a database icon). A disclaimer section follows, stating that the data is test data from an incomplete migration of public data from the FDA and other sources. At the bottom of the browser window, a search bar shows the word 'evolution' and a message from Firefox suggesting a fresh start.

Welcor X NCATS L Connecting l Substanc Welcome ask software pgAdmin Stop (kill) cowsay -\ do cows l /home/welst +

localhost kill sigterm play →

Delta 10" table saw - t... Cabinet/Lockable Ke... 64 bit - WebEx deskto...

ginas ginas G-SRS Software Getting Started Documentation FAQ

# Starting with G-SRS

Download and installation instructions

**G-SRS v2.0** (October 12, 2017)

Download with data

G-SRS v2.0

Download software only

G-SRS v2.0

Download sample data

test 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

evolution ^ v Highlight All Match Case Whole Words 1 of 5 matches

It looks like you haven't started Firefox in a while. Do you want to clean it up for a fresh, like-new experience? And by the way, welcome back! Refresh Firefox... X

# Unzip the downloads

<

>

Home

Documents

ginas2

gsr2.0h2

conf

🔍

☰

⋮

🕒 Recent

🏠 Home

🖥 Desktop

📁 Documents

⬇ Downloads

🎵 Music

📷 Pictures










📺 Videos

🗑 Trash

🌐 Network

💻 Computer

🖨 Connect to Server

Name	Size	Type	Modified
 bin	3 items	Folder	Oct 11 2017
 conf	13 items	Folder	Feb 6
 ginas.ix	6 items	Folder	Oct 11 2017
 lib	167 items	Folder	Oct 11 2017
 logs	5 items	Folder	00:01
 share	1 item	Folder	Oct 11 2017
 access-log-2018-02-06.gz	2.8 kB	Archive	00:01
 application-log-2018-02-06.gz	35.3 kB	Archive	00:00
 RUNNING_PID	4 bytes	Text	Feb 6

# Locate "ginas.conf"

<

>

HomeDocumentsginas2gsr2.0h2**conf**

Q

≡

⋮

Recent

Home

Desktop

Documents

Downloads

Music

Pictures

Videos

Trash

Network

Computer

Connect to Server

evolutions

ginas-legacy-audit.conf

validation.conf

sql

ginas-test.conf

codeSystem.json

ix.ginas.routes

cv.json

kew.json

fda.conf

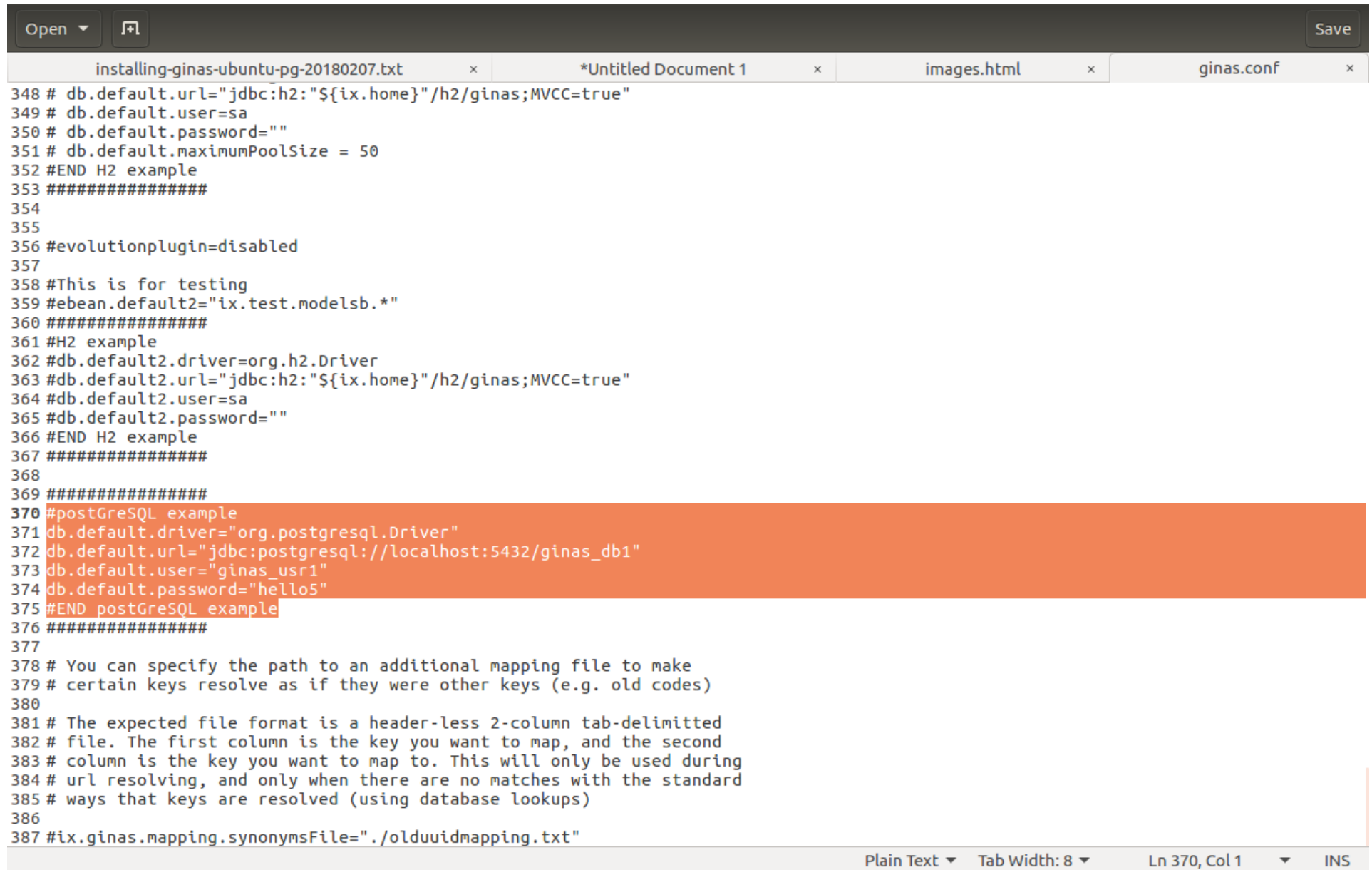
oracleTranslations.txt

ginas.conf

play.plugins

"ginas.conf" selected (9.8 kB)

# Edit "ginas.conf"



```
348 # db.default.url="jdbc:h2:${ix.home}/h2/ginas;MVCC=true"
349 # db.default.user=sa
350 # db.default.password=""
351 # db.default.maximumPoolSize = 50
352 #END H2 example
353 #####
354
355
356 #evolutionplugin=disabled
357
358 #This is for testing
359 #ebean.default2="ix.test.modelsb.*"
360 #####
361 #H2 example
362 #db.default2.driver=org.h2.Driver
363 #db.default2.url="jdbc:h2:${ix.home}/h2/ginas;MVCC=true"
364 #db.default2.user=sa
365 #db.default2.password=""
366 #END H2 example
367 #####
368
369 #####
370 #postgreSQL example
371 db.default.driver="org.postgresql.Driver"
372 db.default.url="jdbc:postgresql://localhost:5432/ginas_db1"
373 db.default.user="ginas_usr1"
374 db.default.password="hello5"
375 #END postgreSQL example
376 #####
377
378 # You can specify the path to an additional mapping file to make
379 # certain keys resolve as if they were other keys (e.g. old codes)
380
381 # The expected file format is a header-less 2-column tab-delimited
382 # file. The first column is the key you want to map, and the second
383 # column is the key you want to map to. This will only be used during
384 # url resolving, and only when there are no matches with the standard
385 # ways that keys are resolved (using database lookups)
386
387 #ix.ginas.mapping.synonymsFile="./olduuidmapping.txt"
```

Plain Text ▾ Tab Width: 8 ▾ Ln 370, Col 1 ▾ INS

# About "apt-get" (installing a package silly example)

```
welscha@kale:~$ sudo apt-get install cowsay
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following packages were automatically installed and are no longer required:
  linux-headers-4.10.0-28 linux-headers-4.10.0-28-generic linux-headers-4.10.0-40 linux-headers-4.10.0-40-generic
  linux-image-4.10.0-28-generic linux-image-4.10.0-40-generic linux-image-extra-4.10.0-28-generic
  linux-image-extra-4.10.0-40-generic
Use 'sudo apt autoremove' to remove them.
The following additional packages will be installed:
  cowsay-off
Suggested packages:
  filters
The following NEW packages will be installed:
  cowsay cowsay-off
0 upgraded, 2 newly installed, 0 to remove and 80 not upgraded.
Need to get 0 B/21.7 kB of archives.
After this operation, 112 kB of additional disk space will be used.
Do you want to continue? [Y/n] Y
Selecting previously unselected package cowsay.
(Reading database ... 291230 files and directories currently installed.)
Preparing to unpack .../cowsay_3.03+dfsg1-15_all.deb ...
Unpacking cowsay (3.03+dfsg1-15) ...
Selecting previously unselected package cowsay-off.
Preparing to unpack .../cowsay-off_3.03+dfsg1-15_all.deb ...
Unpacking cowsay-off (3.03+dfsg1-15) ...
Processing triggers for man-db (2.7.5-1) ...
Setting up cowsay (3.03+dfsg1-15) ...
Setting up cowsay-off (3.03+dfsg1-15) ...
welscha@kale:~$
```

```
welscha@kale:~$ echo "Got Alfalfa?"|cowsay
```

```
< Got Alfalfa? >
```

```
-----  
      \      ^__^  
       (oo)\_____  
            (_____)  \_____  )\/  
                ||----w |  
                ||     ||
```

```
welscha@kale:~$
```

# Install postgres (more complicated but same idea)

```
myuser%> cd
myuser%> mkdir temp-pg
myuser%> cd temp-pg
|
myuser%> wget -q https://www.postgresql.org/media/keys/ACCC4CF8.asc -O - | sudo apt-key add -

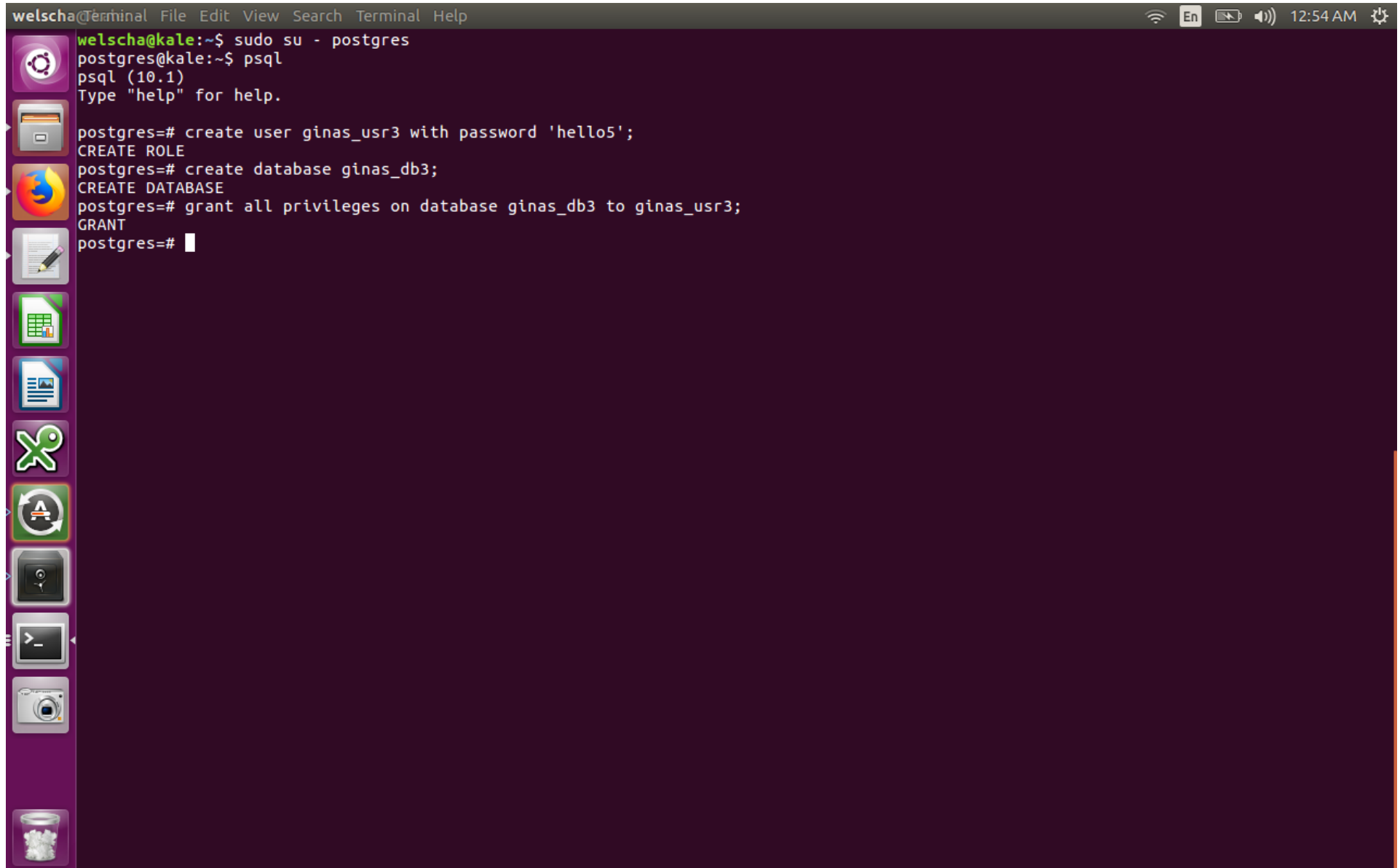
myuser%> sudo sh -c 'echo "deb http://apt.postgresql.org/pub/repos/apt/ `lsb_release -cs`-pgdg main" >> /etc/apt/sources.list.d/pgdg.list'

myuser%> sudo apt-get update
myuser%> sudo apt-get upgrade

myuser%> sudo apt-get install postgresql postgresql-contrib
myuser%> cd
```



# Creating a postgres user and db

A terminal window titled 'welscha@Terminal' with a menu bar (File, Edit, View, Search, Terminal, Help) and a status bar (12:54 AM). The terminal shows the user 'welscha' switching to 'postgres' using 'sudo su - postgres'. Then, 'psql' is launched, showing 'psql (10.1)' and a prompt 'Type "help" for help.'. The user enters 'create user ginas\_usr3 with password 'hello5';', 'CREATE ROLE', 'create database ginas\_db3;', 'CREATE DATABASE', and 'grant all privileges on database ginas\_db3 to ginas\_usr3;'. The terminal ends with 'GRANT' and 'postgres=#' followed by a cursor.

```
welscha@kale:~$ sudo su - postgres
postgres@kale:~$ psql
psql (10.1)
Type "help" for help.

postgres=# create user ginas_usr3 with password 'hello5';
CREATE ROLE
postgres=# create database ginas_db3;
CREATE DATABASE
postgres=# grant all privileges on database ginas_db3 to ginas_usr3;
GRANT
postgres=#
```

# Run ginas!

```
welscha@kale:~/Documents/ginas2/gsr2.0h2$ ./bin/ginas -Dconfig.file=conf/ginas.conf -J-Xmx4G
Play server process ID is 15766
Initializing
█
```

# Import the sample data

Login using admin/admin as credentials; then click on Admin > Data Management

The screenshot shows the G-SRS Job Monitor interface in a Mozilla Firefox browser. The browser's address bar displays the URL `localhost:9000/ginas/app/monitor/2c7e2cfa976a2e483b8e`. The page title is "Job Monitor - Mozilla Firefox". The G-SRS logo and version "2.0.01 beta" are visible in the top left. The top navigation bar includes links for "Browse Substances", "Register Substance", "Structure Search", "Sequence Search", and "Admin". A search bar and a user profile dropdown (showing "admin") are also present. The main content area is titled "Import batch file 'smallSeedData.gsrns'" and is marked as "RUNNING". A gear icon and a "View Records" button are on the left. The progress section shows "Loading data" with a progress bar at 294/10178. Below this, a "Hide Details" button is visible. The progress details are as follows:

Category	Value
Extracted Records	297
Processed Records	296
Persisted Records	294

Summary statistics at the bottom of the progress section:

- Total time running: 4 minutes
- Average Records per second: 1.332
- Estimated time left: 2 hours

A system message at the bottom of the browser window states: "It looks like you haven't started Firefox in a while. Do you want to clean it up for a fresh, like-new experience? And by the way, welcome back!" with a "Refresh Firefox..." button.

# Browse substances

Welcome to NCATS Log Connecting to Substan X Welcome to software in pgAdmin 4 postgres - W cowsay - W do cows lik +

localhost:9000/ginas/app/substances cows like alfalfa

Delta 10" table saw - t... Cabinet/Lockable Ke... 64 bit - WebEx deskto...

## G-SRS

version 2.0.01 beta

Browse Substances Register Substance Structure Search Sequence Search Admin Search ...

admin Logout

Show Deprecated Records ☐

Substance Type

- ☐ Chemical 9871
- ☐ Protein 434
- ☐ Concept 230
- ☐ Structurally Diverse 91
- ☐ Mixture 63

More ...

Molecular Weight

- ☐ 0:200 1565
- ☐ 200:400 5738
- ☐ 400:600 2634
- ☐ 600:800 564
- ☐ 800:1000 215


10744 << < 1 2 3 4 5 6 7 8 ... 671 672 > >>

Sort By: Sort By

### LIATERMIN

PI2EQ4KE3

PROTEIN



**Names:** LIATERMIN  
METHIONYL NEUROTROPHIC FACTOR (HUM...  
N-METHIONYL HUMAN GLIAL CELL LINE-DER...  
لياتارمين  
liatermine

**Codes:** CAS: 188630-14-0  
INN: 7885  
MERCK INDEX: M5680

**Relationships:** 1

**Date approved:** 2 years ago

**Created:** a few seconds ago

**Last modified:** a few seconds ago

**Status:** Validated (UNII)

**Version:** 1

Subunits: 2

It looks like you haven't started Firefox in a while. Do you want to clean it up for a fresh, like-new experience? And by the way, welcome back! Refresh Firefox...

# Looking at the database (optional PgAdmin4)

The screenshot shows the pgAdmin 4 web interface in a browser window. The address bar indicates the connection to `localhost:5050/browser/`. The left sidebar displays the database structure, with the `ix_ginas_name` table selected. The table has 20 columns, including `uuid`, `current_version`, `created`, `created_by_id`, `last_edited`, `last_edited_by_id`, `deprecated`, `record_access`, `internal_references`, `owner_uuid`, `name`, `full_name`, `std_name`, `type`, `domains`, `languages`, `name_jurisdiction`, `preferred`, `display_name`, and `internal_version`.

The right sidebar shows the SQL query editor with the following query:

```
1 SELECT * FROM public.ix_ginas_name
2 ORDER BY uuid ASC
```

Below the query editor, the "Data Output" tab is active, displaying a table with 11 rows of data. The columns are `uuid` (PK) character varying (40) and `current_version` integer.

	uuid [PK] character varying (40)	current_version integer
1	0000f1aa-1337-4cf4-afe3-8775...	
2	0001db5d-b1fb-40a9-a59a-ade...	
3	0004c9e3-d858-4e0a-b8d6-611...	
4	00081894-4641-44ba-9c06-c65...	
5	000ba524-c2f8-459a-9f6c-134a...	
6	000d02df-90c0-4df0-ae98-e6c4...	
7	000d2ff4-1bfe-4669-a22b-840f2...	
8	0010df7e-b1ab-4079-b508-9db...	
9	001146fb-6040-45bb-9ed5-631...	
10	0012539e-9e75-47aa-86fc-5ca6...	
11	00161338-856c-4ebc-9edd-654f...	

At the bottom of the interface, there is a search bar with the text `substn` and a status message: "It looks like you haven't started Firefox in a while. Do you want to clean it up for a fresh, like-new experience? And by the way, welcome back!"

Welcome to...NCATS Login...Connecting to ti...Job Monitor...Welcome to...ask software ins...pgAdmin 4...postgres - Gc...+

localhost:5050/browser/istall with apt get →

pgAdmin 4FileObjectToolsHelp

BrowserDashboardPropertiesSQLStatisticsDependenciesDependentsEdit Data - localh...Edit Data - localh...Edit Data - localhost - ginas\_...

100 rows

localhost - ginas\_db1 - public.ix\_ginas\_name

1SELECT \* FROM public.ix\_ginas\_name

2ORDER BY uuid ASC LIMIT 100

3

Data Output

ExplainMessagesQuery History

edited_by_id	deprecated boolean	record_access bytea	internal_references text	owner_uuid character varying (40)	name character varying (255)	full_name text	std_name text	type character varying (3
1	false	[binary data]	[{"label": "GlnAS Referen...	818be705-47c1-449c-a5c4...	amcinonidum	[null]	amcinonidum	of
1	false	[binary data]	[{"label": "GlnAS Referen...	15c546df-5b29-407f-8e0c...	DIPIVALYL EPINEPHRINE	[null]	DIPIVALYL E...	cn
1	false	[binary data]	[{"label": "GlnAS Referen...	7d440c45-03fe-4e80-a845...	1-(5-HYDROXY-5-METHYLH...	[null]	1-(5-HYDRO...	sys
1	false	[binary data]	[{"label": "GlnAS Referen...	8fdb8390-7a89-48e2-a731...	tioperidona	[null]	tioperidona	of
1	false	[binary data]	[{"label": "GlnAS Referen...	6f70cd8-8080-43f7-a7cb...	بريکينار	[null]	بريکينار	of
1	false	[binary data]	[{"label": "GlnAS Referen...	2c1c0e3a-44fa-4b73-bce6...	بانينولينز	[null]	بانينولينز	of
1	false	[binary data]	[{"label": "GlnAS Referen...	1ec43b3a-2ee8-446e-952...	inosina	[null]	inosina	of
1	false	[binary data]	[{"label": "GlnAS Referen...	af5343a7-c1bc-4950-bd4d...	苯味洛尔	[null]	苯味洛尔	of
1	false	[binary data]	[{"label": "GlnAS Referen...	358f7845-5bba-4837-93db...	1-CYCLOHEXYL-3-(P-(2-(1-E...	[null]	1-CYCLOHE...	cn
1	false	[binary data]	[{"label": "GlnAS Referen...	d9b92dde-8875-4e8e-9bb...	isoxsuprina	[null]	isoxsuprina	of
1	false	[binary data]	[{"label": "GlnAS Referen...	701fe7ee-76a2-48a5-8373...	MALARONE COMPONENT A...	[null]	MALARONE ...	cn

substn

Highlight AllMatch CaseWhole WordsPhrase not found

It looks like you haven't started Firefox in a while. Do you want to clean it up for a fresh, like-new experience? And by the way, welcome back!

Refresh Firefox...

# Kill the ginas process

```
welscha@kale:~/Documents/ginas2/gsr2.0h2$ ./bin/ginas -Dconfig.file=conf/ginas.conf -J-Xmx4G
Play server process ID is 15766
Initializing
welscha@kale:~/Documents/ginas2/gsr2.0h2$
```

In another terminal window ...

```
welscha@kale:~$
welscha@kale:~$
welscha@kale:~$ kill -SIGTERM 15766
welscha@kale:~$
```

# Details with CLI commands

INSTALLING THE GINAS, PUBLIC VERSION ON UBUNTU 16.04  
USING POSTGRESQL 10 AS DATABASE

Ginas Monthly Meeting  
Feb 7th, 2017  
Alex Welsch

```
=====
*** STEP 1. Get background information and instructions on the NCATS site
=====
```

<https://tripod.nih.gov/ginas/#/gsrs/release>

(There are instructions if you scroll down!)

Requirements:

- 4-core (+) CPU
- 8GB (+) Memory
- 100GB (+) hard drive
- Java 8

For our purposes, the evolutions step should be skipped.

```
=====
*** STEP 2. Download the public Ginas version and example data.
=====
```

See: <https://tripod.nih.gov/ginas/#/gsrs/release>

Open a linux terminal window and issue the following commands:

```
myuser%> cd
myuser%> mkdir ginas2
myuser%> cd ginas2
myuser%> wget https://tripod.nih.gov/ginas/releases/gsrs2_0_beta_bundled_h2_smallseed.zip
myuser%> unzip gsrs2_0_beta_bundled_h2_smallseed.zip
myuser%> wget https://tripod.nih.gov/ginas/releases/smallSeedData.gsrs
myuser%> cd gsr2.0h2
myuser%> ls # to see contents
```

```
=====
*** STEP 3. INSTALL POSTGRESQL
=====
```

(From: <https://tecadmin.net/install-postgresql-server-on-ubuntu/>)

```
myuser%> cd
myuser%> mkdir temp-pg
myuser%> cd temp-pg
```

```
myuser%> wget -q https://www.postgresql.org/media/keys/ACCC4CF8.asc -O - | sudo apt-key add -
```

```
myuser%> sudo sh -c 'echo "deb http://apt.postgresql.org/pub/repos/apt/ `lsb_release -cs`-pgdg main"
>> /etc/apt/sources.list.d/pgdg.list'
```

```
myuser%> sudo apt-get update
myuser%> sudo apt-get upgrade
```



```
myuser%> sudo apt-get install postgresql postgresql-contrib
myuser%> cd
```

## If all goes well, a linux operating system "postgres" user now exists.

```
myuser%> sudo su - postgres
==> gets you to that account temporarily.
```

```
postgres%> exit
==> to get back to your own user account.
```

```
myuser%>
```

## Go back into the postgres account and start "psql" --- the command line interface.

```
myuser%> sudo su - postgres
postgres%> psql
postgres=# \password postgres    ## I set it to hello4
postgres=# \q
```

```
=====
*** STEP 4. Create the Ginas database and database user
=====
```

```
postgres%> psql
```

```
## You're now in the postgres CLI.
## Issue the following commands to create a Ginas user and database.
## You can use whatever user/database/password you want.
```

```
postgres-# create user ginas_usr with password 'hello5';
postgres-# create database ginas_db;
postgres-# grant all privileges on database ginas_db to ginas_usr;
postgres-# \q
postgres%> exit
myuser%>
```

```
=====
*** STEP 5. MAKE Postresql open to local accounts on the computer.
=====
```

## Change your PostresSQL configuration to allow local access to the Postgresql database.

```
myuser%> sudo nano /etc/postgresql/10/main/pg_hba.conf
```

```
## Change the Posgres Configuration to allow local connections
```

```
## Chnage FROM:
```

```
    local    all        all        peer
```

```
## TO:
```

```
    local    all        all        md5
```

```
## Control-X to quit nano.
```

```
## then restart Postgresql Server
```

```
myuser%> sudo service postgresql restart
```

## Now, check if we can access database with psql. Notice we are doing it directly from myuser%

```
myuser%> psql -U ginas_usr -d ginas_db -W
ginas_db=>
```

```
## try \l to list databases, the quit.
```

```
ginas_db=> \l
ginas_db=> \q
```

```
=====
*** STEP 6.  Change your ginas configuration to specify PostgreSQL.
=====
```

```
myuser%> cd
myuser%> cd ginas2/gsr2.0h2
myuser%> nano ./conf/ginas.conf
```

Add the following at the END.

```
#postGreSQL example
db.default.driver="org.postgresql.Driver"
db.default.url="jdbc:postgresql://localhost:5432/ginas_db"
db.default.user="ginas_usr"
db.default.password="hello5"
#END postGreSQL example
```

```
=====
*** STEP 7.  Run Ginas
=====
```

```
myuser%> ./bin/ginas -Dconfig.file=conf/ginas.conf -J-Xmx4G
## ... or
myuser%> nohup ./bin/ginas -Dconfig.file=conf/ginas.conf -J-Xmx4G
```

## Take note of the process ID after so you can stop it later.

## When the program is done initializing ==> in your browser load:

<http://localhost:9000/ginas/app>

## Click on the Admin link, login with credentials.

```
    user: admin
    password: admin
```

## If this is your first time, you'll have no data and you'll have to import it.

a) click on admin in the TOP menu (next to "sequence search")  
b) click on data management  
c) In the file dialog, navigate to the file smallSeedData.gsr.s you downloaded earlier and click on the load button. Loading will take a while. You don't have to load everything if you just want to see if it worked. After loading some substances, you'll be able to browse substances by clicking on the Substances Link.

```
=====
*** STEP 7.  Quit Ginas
=====
```

## When you want to end the process gracefully:

```
myuser%> kill -SIGTERM YOUR_PROCESS_ID
```

```
=====
*** ERRORS YOU MIGHT GET
=====
```

In some attempts, the Play framework seemed to hang or complained about file locks. I made things work by clearing the cache directory (./ginas.ix/cache). However, there maybe consequences contend with if you do that.

Database 'default' is in an inconsistent state with postgresql driver.  
==> I got this when I first tried to install and maybe things didn't complete with the database population. The remedy was to drop the database and recreate it as in Step 4

Oops, cannot start the server.  
org.jboss.netty.channel.ChannelException: Failed to bind to: /0.0.0.0:9000  
==> find the PID for the process running play framework with ==> ps auxwww | grep play ==> then ==> kill -9 YOUR\_PID

After running ginas, screen hangs and says "Initializing" forever.  
(It may not tell you it's done initializing, so if you've been staring at a blank screen that says "initializing" for a while, try loading <http://localhost:9000/ginas/app> in your server. )

=====  
\*\*\* Links  
=====

<https://tripod.nih.gov/ginas/#/gsrs/>

<https://help.ubuntu.com/community/AptGet/Howto>

<https://medium.com/coderscorner/installing-oracle-java-8-in-ubuntu-16-10-845507b13343>

<https://tecadmin.net/install-postgresql-server-on-ubuntu/>

<http://suite.opengeo.org/docs/latest/dataadmin/pgGettingStarted/firstconnect.html>

<https://www.ntchosting.com/encyclopedia/databases/postgresql/create-user/>

<http://blog.jasonmeridth.com/posts/postgresql-command-line-cheat-sheet/>

<https://askubuntu.com/questions/831262/how-to-install-pgadmin-4-in-desktop-mode-on-ubuntu>  
(see Victor's answer)

```
Once you've installed it, start it again, like so:
## cd ~/pgadmin4
## source bin/activate
## python lib/python2.7/site-packages/pgadmin4/pgAdmin4.py
```

<https://www.digitalocean.com/community/tutorials/sqlite-vs-mysql-vs-postgresql-a-comparison-of-relational-database-management-systems>

=====  
\*\*\* Explore API  
=====

<https://tripod.nih.gov/ginas/#/gsrs/api#details>

<https://tripod.nih.gov/ginas/app/api/v1>