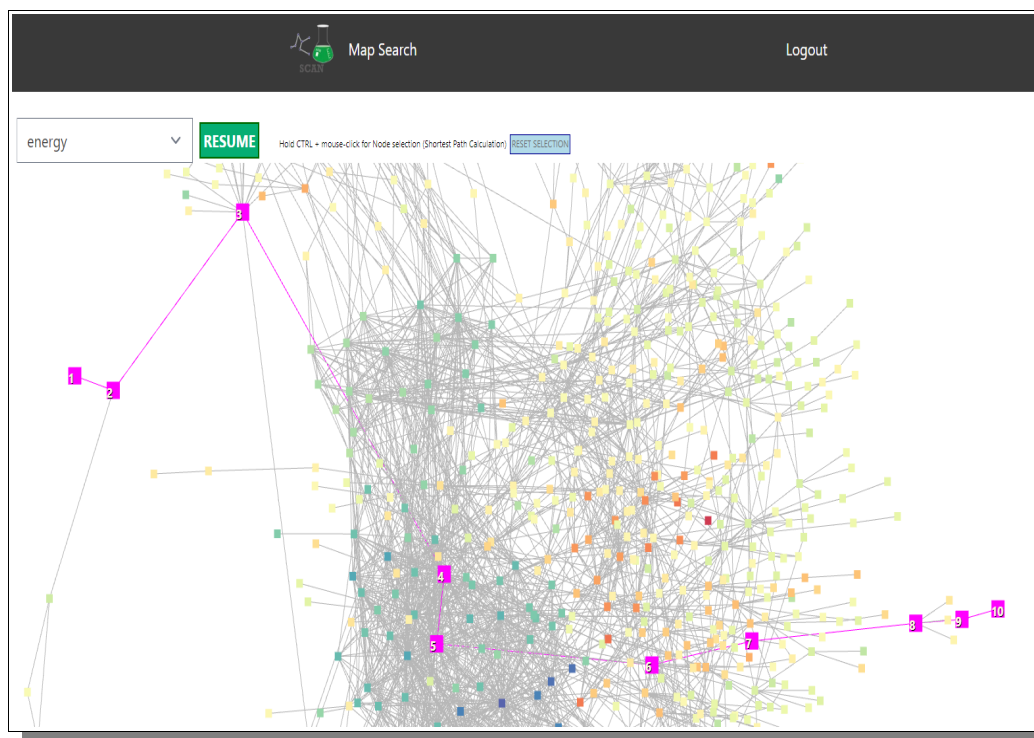


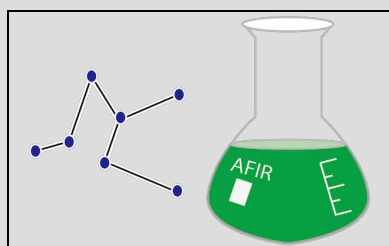


TAKAHASHI GROUP (情報化学研究室)

Hokkaido University



WEB APPLICATION FOR SEARCHING CHEMICAL ACTIONS AND NETWORKS



# SCAN

# Server Setup Manual

*ENGLISH ORIGINAL*

# SCAN Server Setup Manual

---

## CONTRIBUTORS

### SCAN System Developers

Micke Nicander Kuwahara  
Jun Fujima

*This document was last updated  
April 17, 2023 14:00*

### SCAN Web Application

[Searching Chemical Actions and Networks]

Copyright © 2018 Keisuke Takahashi, Micke Nicander Kuwahara  
in Takahashi Group (情報化学研究室) of Hokkaido University

\*\*\*\*\*

SCAN is licensed under the GNU GPL License, Version 3.0;  
you may not use this file except in compliance with the License.  
You may obtain a copy of the License at

<https://www.gnu.org/licenses/gpl-3.0.en.html>

Unless required by applicable law or agreed to in writing, software  
distributed under the License is distributed on an "AS IS" BASIS,  
WITHOUT WARRANTIES OR CONDITIONS OF ANY KIND, either express or implied.  
See the License for the specific language governing permissions and  
limitations under the License.

For any further information, visit the project GitHub at

<https://github.com/scan-team/scan-platform-test>

\*\*\*\*\*

Takahashi Group  
Hokkaido University, Faculty of Science, Department of Chemistry,  
7th building, Room 7-510, Kita 10, Nishi 8, Kita-ku,  
Sapporo, 060-0810, Japan.  
[scan-team@sci.hokudai.ac.jp](mailto:scan-team@sci.hokudai.ac.jp)

# Table of Contents

CONTRIBUTORS.....	1
Table of Contents.....	2
Preface.....	3
Introduction.....	4
SCAN Architecture.....	4
Web-based Browsing Interface.....	5
Server Setup Manual.....	6
Prerequisites.....	6
Preparing the Environment.....	7
Setting up and configuring an Auth0 account.....	7
Scan Server Configuration.....	10
Getting SCAN from Github.....	11
Creating and editing SCAN project configuration files.....	11
Scan Server Build and Startup.....	13
Data Registration Procedure.....	15
Registration of sample data.....	15
Summary.....	15
Index.....	16
Figure Index.....	16
Table Index.....	16

# Preface

*A few words from the creators.*

This manual is attempting to be an extensive guide to anyone who wishes to setup their own public SCAN Server found online at GitHub at <https://github.com/scan-team/scan-platform-test>. The interactive chemical reaction platform, SCAN, is developed for analyzing chemical reaction networks. SCAN offers the chemical reaction path network database, visualization, and network analysis tools. In particular, SCAN is a web-based platform that allows users to perform interactive chemical reaction path network visualization and data science techniques with simple operation. SCAN is designed to provide a user-friendly graphic user interface, making preexisting knowledge of programming and skill sets optional. Thus, SCAN is proposed to be an alternative tool for analyzing and understanding chemical reaction networks.

SCAN is basically a visualization and analyzing tool for network data, with exclusive focus on chemical reaction data. SCAN was originally mainly developed to use AFIR data, but that is not a limitation chiseled in stone. Any developer who downloads the SCAN code and server setup manual are free to alter the database as one sees fit and use any data they like.

So to be clear, the SCAN software development team is not involved in choosing and uploading the data, and we do not take any responsibility for the data content. Our only focus is the toolsets and the things one can do with the data chosen.

For any AFIR data related issues, please contact the iCreDD (<https://www.icredd.hokudai.ac.jp>) team at Hokkaido University (lead by Professor Satoshi Maeda).

April 17, 2023

*SCAN Software Project Leader*

*Director of Takahashi Group - Information Chemistry Laboratory*

Professor Keisuke Takahashi

*SCAN Software System Lead Developer*

Micke Nicander Kuwahara

## Introduction

*Get to know what SCAN is and what it can do for you as a researcher and chemist.*

Understanding the chemical reaction answers the fundamental mystery of how products are formed from reactants. First principle calculations unveil that the chemical reaction is a complex matter as it involves a tremendous number of intermediates. In other words, a chemical reaction can be treated as a form of a complex network consisting of numerous molecular interactions. While it is difficult to capture the details of molecular interactions in an experiment, first principle calculations play a major role in understanding such a complex reaction map. In particular, numerous automatic chemical reaction searching tools have been developed such as freezing string method with the Berny algorithm, single/double-ended growing string methods, artificial force induced reaction (AFIR), reaction mechanism generator (RMG), and kinbot. Although such complex reaction networks become available, the question arises over how such complex networks can be understood and how knowledge can be extracted, rendering tools for extracting the knowledge from networks necessary.

Extracting knowledge from the chemical reaction network involves multiple steps and processes. In particular, organization of chemical reaction database, statistical analysis, network visualization, and graph theory are involved. Several network visualization tools are available such as Cytoscape and Gephi which offer network visualization and graph theory analysis. Moreover, it has been demonstrated that graph theory such as centrality analysis is found to be effective when determining intermediates. However, these processes are strongly linked to each other, meaning that the individual development of each process could limit the ability to extract knowledge. In addition, network data visualization and analysis often require particular skillsets as well as advanced programming skills, which can act as barriers towards performing such analyses. Therefore, it is crucial to establish a centralized, interactive, and user-friendly platform which has the ability to utilize these processes simultaneously. Here, Searching Chemical Action and Network (SCAN) is introduced where a platform for interactive chemical reaction network is designed and proposed where chemical reaction network produced by the AFIR method. The SCAN platform is available at <https://scan.sci.hokudai.ac.jp/> where it offers the users to explore, visualize and analyze the chemical reaction network data generated by the first principle calculation. Thus, SCAN offers the search and understand the complex chemical reaction network.

### SCAN Architecture

The concept of SCAN is to store and share the chemical reaction network generated by the first principle calculation where interactive network visualization and network analysis are also provided. In order to achieve the flexible reuse of data, the layered architecture consists of a data lake, data warehouse, and data mart. Here, chemical reaction network generated by AFIR methods is used as a prototype chemical reaction network data where data is previously published. The chemical reaction network data generated by AFIR contains numerous log files which are classified as raw data. These raw

## SCAN Server Setup Manual

data are stored in their original form with no modifications. This data storage unit is defined as a data lake. The raw data provided by the data lake is then preprocessed for network visualization and network analysis and stored in a data warehouse. Lastly, the data warehouse is accessed by the data mart, which provides application services such as data visualization, data analysis, and an application programming interface for data sharing.

### Web-based Browsing Interface

Web applications are constructed where the three-layered architecture are used as the foundation. The web application directly connects to the data mart, which allows the user to directly access the web graphic user interface to carry out network visualization, network analysis, and data downloading without previous experience with programming or data preprocessing. This is particularly attractive as it expands access to chemical reaction analysis to researchers that may not have the knowledge or skillsets required for such research.

Map Search Logout

---

Map Search

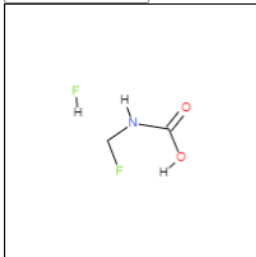
atoms ▼

Sort:  ▼      Order:  ▼

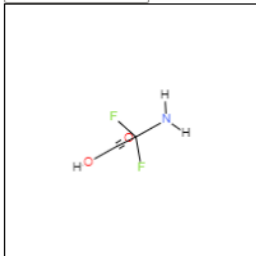
**SEARCH**

---

Results: 14 map found.



[OC\(=O\)C\(F\)\(F\)N](#)  
**Id:** 01GP0GY4CJ35799A4K1TTYJ68R  
**Atoms:** C,O,O,H,N,H,H,C,F,F  
**Lowest\_energy:** -482.440709102611  
**highest\_energy:** -481.838406291197  
**EQs:** 1765, **TSs:** 6526  
Created: January 5, 2023  
Updated: January 5, 2023



[OC\(=O\)C\(F\)\(F\)N](#)  
**Id:** 01GP0H20WYRYEQ8EJBK0KHV347  
**Atoms:** C,O,O,H,N,H,H,C,F,F  
**Lowest\_energy:** -482.275795362779  
**highest\_energy:** -481.885083146466  
**EQs:** 1231, **TSs:** 6714  
Created: January 5, 2023  
Updated: January 5, 2023

# Server Setup Manual

*So you have visited SCAN online and you have a feeling that it may be what you are looking for, but you want to have your own server. Well, then you are at the right place, because here we will help you download and install your own SCAN server.*

**I**n this chapter we will try to explain everything that you need to know about installing and setting up your own SCAN server environment for both local and public use. There are quite a lot of things to do and it can be quite a daunting task. But hopefully with this manual you are going to be all fine. So let's get to it.

## Prerequisites

Before you even start looking in the direction of SCAN you first need to make sure your system is ready for this. The following preparations are required prior to the implementation of any SCAN Server as further explained in this document.

1. A computer with Ubuntu or Linux OS, with the following systems installed and running:
  - a) Docker and Docker-Compose
    - It's not within the scope of this document to explain anything about Docker, so that will be all on you, but here is a link to start if you do not already have Docker.
    - <https://www.docker.com>
  - b) Python3
    - It's not within the scope of this document to explain anything about Python either, but we guess you know where to go and find out what you need about it online.
2. *[Only for public server, not needed for local version]:*
  - a) *Obtain a domain name for your SCAN app and register it in the DNS*
  - b) *Obtain proper SSL certificate*
  - c) *Register for a Google Analytics ID (optional and how to is not within the scope of this document)*

## Preparing the Environment

After you have made sure that your computer has the required foundation, it is time to install and configure all of the necessities and parts that SCAN needs to run.

### Setting up and configuring an Auth0 account

In this section we will explain how you create an account for the auth0 authentication server which is needed to create and manage user accounts for the SCAN web platform.

- 1) Go to <https://auth0.com> in your browser.

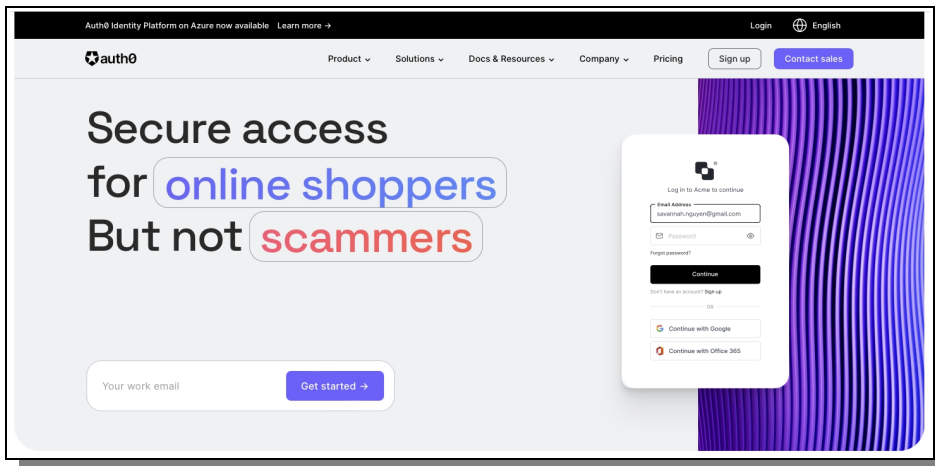


Figure 1: The front page of the Auth0 website that will be your user accounts manager

- 2) Click on the “Sign Up” button to go to the user registration page in the top right section as seen in Figure 1.
- 3) Enter your e-mail address and then click Continue to go to the account creation screen. Enter your password and click Continue. This can be seen below in Figure 2.

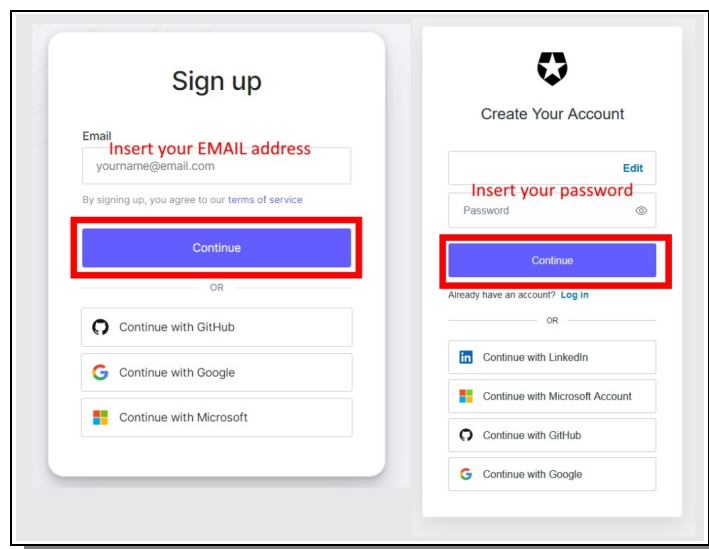


Figure 2: To create a basic User Manager account with Auth0 is free



## SCAN Server Setup Manual

- 4) Select "Account Type", "Company Name" and "Company Size" and click "Next". Confirm "Tenant Domain" and "Region" and click "Create Account" to create the account as seen in Figure 3.

Account Type

Are you creating this account for yourself or on behalf of a company?

Company  Personal

Select Personal or Company

Company Name

Your company name

Enter Company Name

Company Size

1-49 50-200 201-999 1000+

Select Company Size

I need advanced settings

We've assigned your data region to the United States and given you a tenant name. Check this box if you need to process your data in a different region to comply with privacy laws.

Tenant Domain

.us.auth0.com

Confirm Domain Name

To help you easily explore our product, we've selected a tenant domain name for you. Although you can't rename a tenant, you can always add more tenants to your account (for staging or production environments) later.

Region

AU EU Japan US

We can host all of your data in any of these regions. Useful if you need to comply with EU Data Protection Directive

Create Account →

NEXT

Figure 3: The domain name is needed to be obtained before you get here in the process.

- 5) After you have signed up, the dashboard page will be displayed as can be seen in Figure 4.

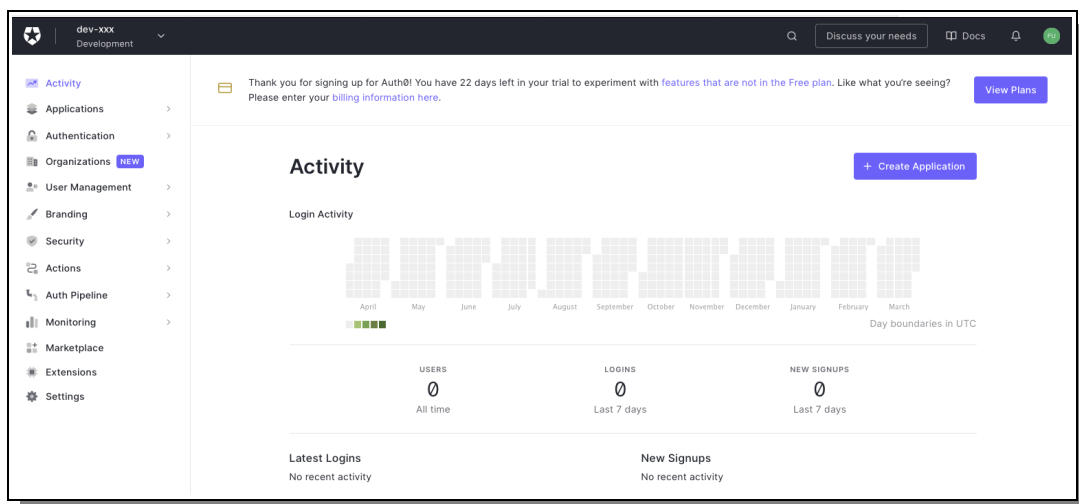


Figure 4: In the Auth0 Dashboard you can now configure the login system for your SCAN server.

- 6) Click "Applications" at the top left of that screen, followed by a click on "Applications" directly below. After that, in the new view in the main area, click "Default App" in order to to move to the setting screen. What was just described can be seen in Figure 5 below.

# SCAN Server Setup Manual

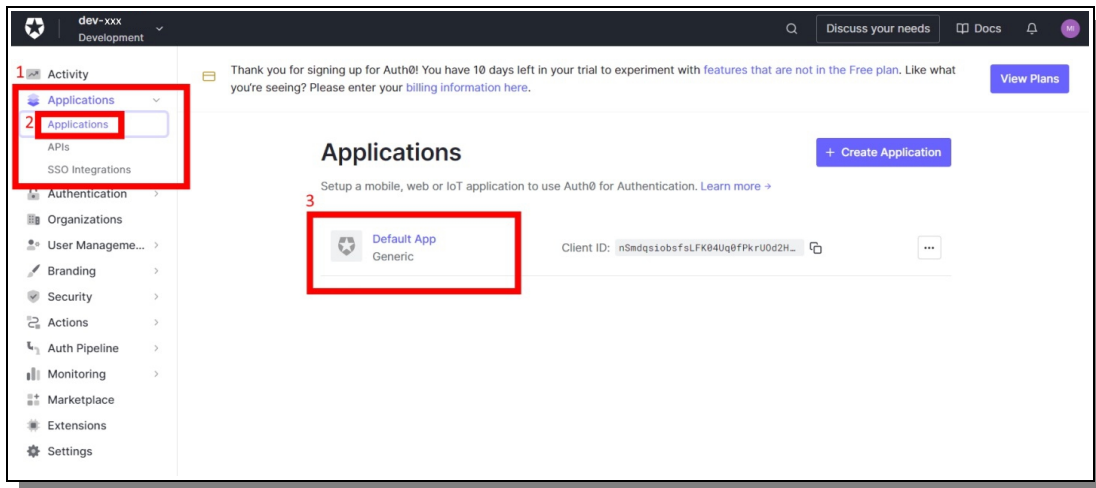


Figure 5: Click yourself to the Default App configuration view.

- 7) Under the Settings tab you will find the parts you need to fill in by scrolling down as shown in Figure 6.

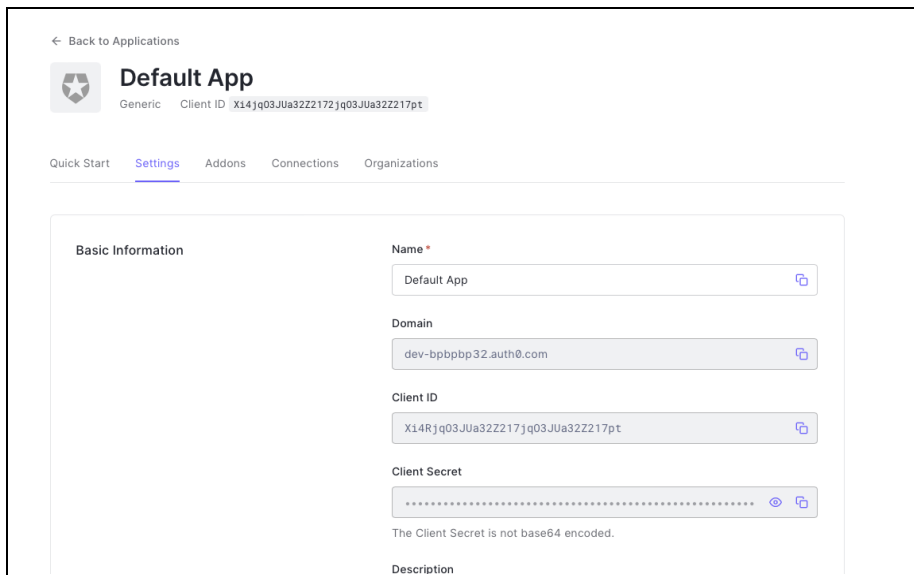


Figure 6: Scroll down in this view to get to the parts that need to be changed or added.

- 8) Enter the URL of the SCAN server in the “Application Login URI” field, found by scrolling further down on the settings page. In Figure 7 you can see the field in question.

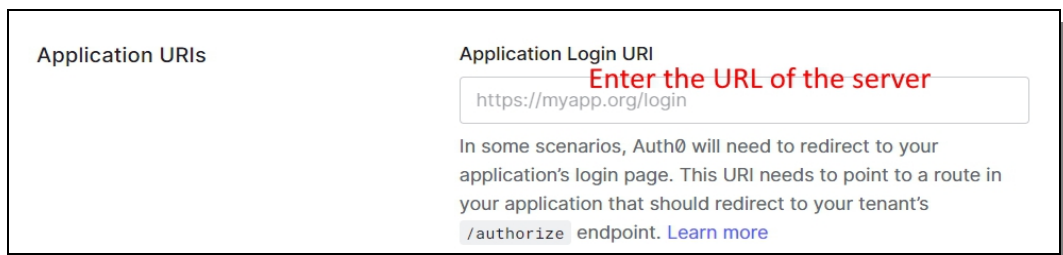
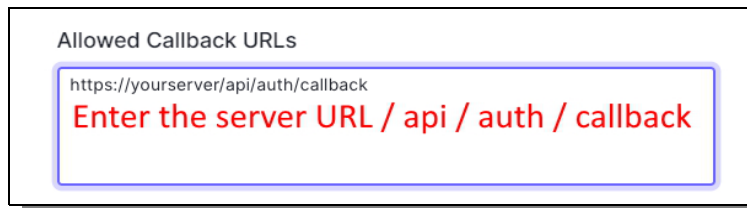


Figure 7: Make sure you have properly registered the url before this step.

## SCAN Server Setup Manual

- 9) Next scroll down to "Allowed Callback URLs" and in that field enter "the Server URL/api/auth/callback" as indicated in Figure 8.



Allowed Callback URLs

https://yourserver/api/auth/callback

Enter the server URL / api / auth / callback

Figure 8: Type in the same url as before, but with the additional path.

- 10) Below the above section can be found the "Allowed Logout URLs". In that field just add the server URL as noted in Figure 9.



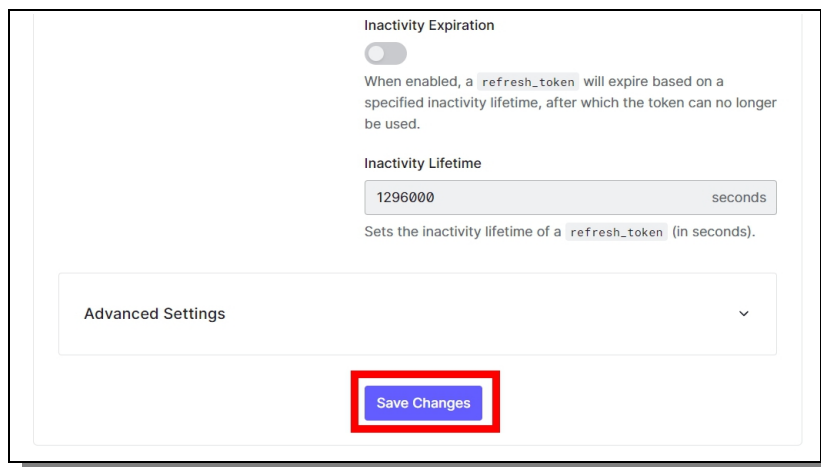
Allowed Logout URLs

https://scan.example.net

Enter the server URL

Figure 9: Just fill in the same URL as before with no additional paths.

- 11) When you're done, scroll down and click 'Save Changes' at the bottom of the screen as seen in Figure 10.



Inactivity Expiration

When enabled, a `refresh_token` will expire based on a specified inactivity lifetime, after which the token can no longer be used.

Inactivity Lifetime

1296000 seconds

Sets the inactivity lifetime of a `refresh_token` (in seconds).

Advanced Settings

Save Changes

Figure 10: Save the settings and then you are ready to go.

## Scan Server Configuration

In this section we are downloading the SCAN code to your server and help you setting it up and configuring it the way it need to be configured in order to run. We will assume that you are familiar with the OS (Linux or Ubuntu) that your are working with, as well as GitHub in general, since none of those parts will be explained further in any details within the scope of this documentation. If you do not master any of those at any good-enough level, then we suggest you go online and find a tutorial and learn.

## SCAN Server Setup Manual

### Getting SCAN from Github

- 1) Log in to the Linux server you are installing to, as the admin user and go to the location in the file system where your SCAN server will reside.
- 2) Make a quick visit to the GitHub page for SCAN at <https://github.com/scan-team/scan-platform-test>, this is the project we will clone and work with. Also take a quick glance at the ReadMe to make sure all looks on par with this documentation. (The ReadMe is updated first if changes occur so if something different is stated there, that is what goes)
- 3) Clone the SCAN repository from GitHub to your server.

```
$ git clone https://github.com/scan-team/scan-platform-test.git my-scan
$ git submodule update --init --recursive
```

- 4) After the SCAN project has finished downloading from GitHub to your server, navigate to the root of the project if you are not already there.

### Creating and editing SCAN project configuration files

- 5) Create a copy of the .env.sample file, found at the root, and name the copy .env

```
$ cd my-scan/
$ cp .env.sample .env
```

- 6) Open the .env file for editing (using your preferred code/text editor) and make the changes required as seen in Figure 11, and as listed with description and example in the Table 1 below.

Item Name	Description	Example
API_ALLOWED_HOSTS	API accessible URL Specify the URL of the server	<i>https://yourhostname:8001/</i>
AUTH0_SECRET	Please specify a random character string.	<i>Oi2Aich1theace6jaiyoekae3aethuizuoz</i>
AUTH0_BASE_URL	Server URL	<i>https://yourhostname/</i>
AUTH0_ISSUER_BASE_URL	Look at AUTH0 application settings: Domains	<i>https://xxx.auth0.com</i> <i>(xxx is found in Auth0 Domain)</i>
AUTH0_CLIENT_ID	Look at AUTH0 application settings: ClientID	
AUTH0_CLIENT_SECRET	Look at AUTH0 application settings: ClientSecret	
NEXT_PUBLIC_SCAN_API_PROXY_ROOT	Add api / proxy to server URL	<i>https://yourhostname/api/proxy</i>
FASTAPI_SIMPLE_SECURITY_SECRET	API access key (for management) Please specify a random string	<i>caaph5eicahneewuiKei3peeVe8shi3I</i>
NEXT_PUBLIC_GOOGLE_ANALYTICS_ID	Specify the measurement ID for data collection with Google Analytics.	<i>G-X3ZZ5HVYYZ</i>

Table 1: These are the environment variables that need to set properly.

## SCAN Server Setup Manual

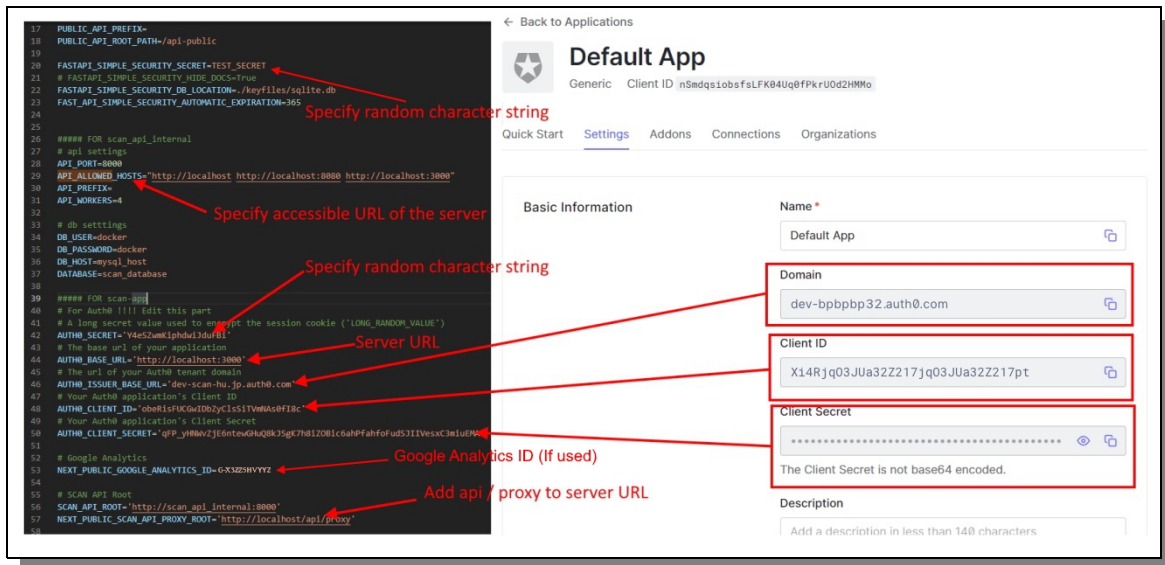


Figure 11: Configuring the .env file in the project root folder correctly is an important part.

- 7) Create a copy of nginx.conf.example from the scan-reverse-proxy/conf.d/directory and name it nginx.conf

```
$ cp nginx.conf.example nginx.conf
```

- 8) Open the nginx.conf file for editing (using your preferred code/text editor) and make the changes required as seen in Figure 12, and as listed with description and example in the Table 2 below.

Item Name	Description	Example
ssl_certificate	SSL certificate file name <sup>1</sup>	/etc/ssl/certs/cert.pem
ssl_certificate_key	SSL private key file name	/etc/ssl/certs/server.pem

Table 2: The SSL certificate keys needs to be registered

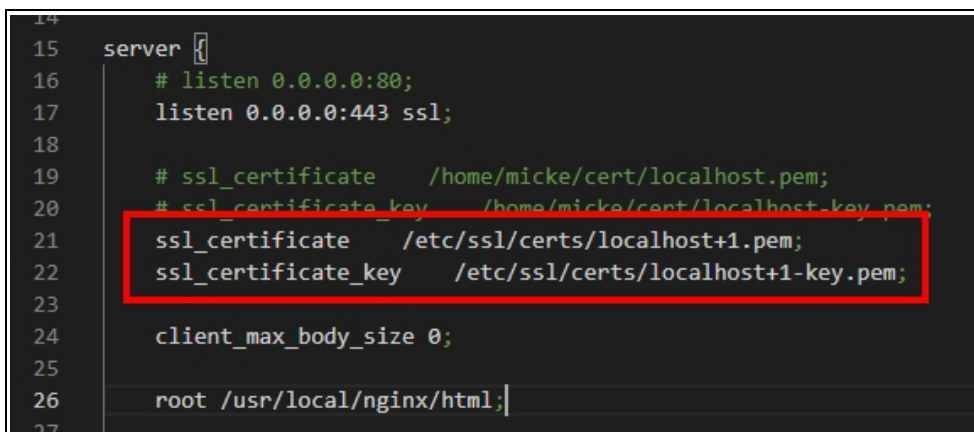


Figure 12: Change the names to point at the SSL key location of your computer

<sup>1</sup>No need to change the path part /etc/ssl/certs (those will be pointed correctly at in docker-compose.yml below)

## SCAN Server Setup Manual

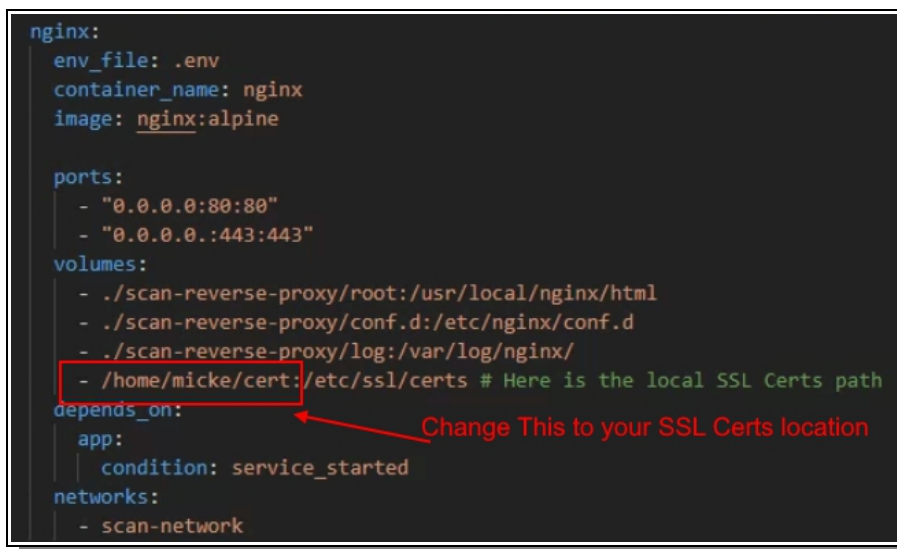
- 9) Create a copy of `docker-compose.yml.example` from the SCAN root folder and name it `docker-compose.yml`

```
$ cp docker-compose.yml.example docker-compose.yml
```

- 10) Open the `docker-compose.yml` file for editing (using your preferred code/text editor) and make the changes required as seen in Figure 13, and as listed with description and example in the Table 3 below.

Item Name	Description	Example
nginx: volumes: -	Repoint the path of your local ssl to the virtual path used by nginx.	YourSSLPath: /etc/ssl/certs

Table 3: Make sure you find the correct local location of the SSL certs



```
nginx:
  env_file: .env
  container_name: nginx
  image: nginx:alpine

  ports:
    - "0.0.0.0:80:80"
    - "0.0.0.0:443:443"

  volumes:
    - ./scan-reverse-proxy/root:/usr/local/nginx/html
    - ./scan-reverse-proxy/conf.d:/etc/nginx/conf.d
    - ./scan-reverse-proxy/log:/var/log/nginx/
    - /home/micke/cert:/etc/ssl/certs # Here is the local SSL Certs path

  depends_on:
    app:
      condition: service_started

  networks:
    - scan-network
```

Figure 13: Your local location of the SSL certs

## Scan Server Build and Startup

Now we have come to the project building and starting part of the documentation where we will execute the Docker build process and see the SCAN server run for the first time.

- 1) Make sure that you are at the project root folder and then execute the build script.

```
$ ./build.sh
```

- 2) Now the docker build process will start, and that may take some time, many minutes perhaps. During that process, information on the process will be written into the terminal in various colors, including red, but all should be well. At the end when all is finished there should be a message that things have been successful.
- 3) If something fails, make sure to double check that you have done all previous parts up to this point correctly. Read the error message and compare with the GitHub ReadMe file that all seem okay. Google the error message if this documentation is not sufficient. After correcting any possible mistake, run the build command above one more time.

## SCAN Server Setup Manual

- 4) After the Docker build process has finished successfully it is time to start the SCAN server via the start script.

```
$ ./start.sh
```

- 5) This process too will take time and a lot of messages will be printed to the terminal, but if all goes well, as it should, at the end all docker containers started and running will be displayed with a green 'Done' as seen in the Figure 14 below.

```
Creating scan_redis      ... done
Creating mysql_host     ... done
Creating scan_app       ... done
Creating test_phpmyadmin ... done
Creating scan_api_internal ... done
Creating scan_api_public ... done
Creating nginx          ... done
```

Figure 14: This is the view you want, showing that the system is all up and running as it should.

- 6) Now go to your browser and open up the website. If it is running with localhost then use that, otherwise use the ip or URL that you have assigned during the configuration. (If you are accessing your server remotely or for some reason can not use localhost, you must make sure to update all links in .env and Auth0.com accordingly with your requested IP settings)
- 7) If all works as intended then you should see the website start page in your browser as seen in Figure 15 below, with the difference that there are zero maps available, that we need to add in the next step.

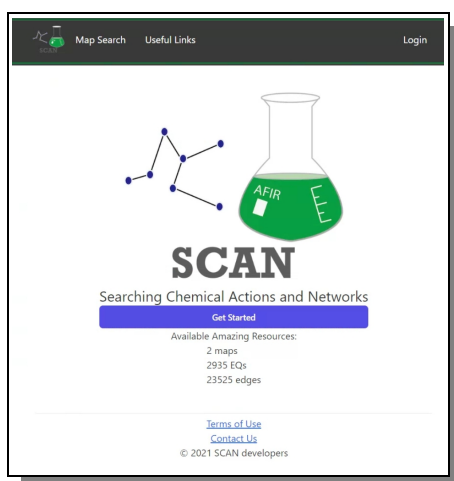


Figure 15: The SCAN website start page

- 8) The 'Terms of Use' link and the 'Contact Us' link will most likely contain wrong information for your setup, so please locate those files and edit them to your liking before deploying online.
- 9) If you later want to stop the server just execute the stop script, and wait for the server to finish.

```
$ ./stop.sh
```



### **Data Registration Procedure**

This section describes the procedure for registering sample data. If you are planning to run your own data or GRRM (AFIR) data or in any other way alter the DB, then perhaps do that later after you made sure that the sample data work fine.

#### **Registration of sample data**

You can load the demo sample data into the database. The following two reaction pathway networks for urea synthesis are registered.

- Wöhler 's urea
- Synthesis

- 1) Download the sample data from the following URL, name it “export.sql”, and upload it to the SCAN server.

<https://drive.google.com/file/d/1VjsEwVdje4G1Ob1fEesMRXmRQRBaajr1/view?usp=sharing>

[if the link is not working, go to SCAN GitHub and locate a proper link there]

- 2) Register the sample data to the database. (make sure the paths and location of the export.sql is correct according to your computer.)

```
$ scan-mariadb/import.sh ../export.sql
```

- 3) This might take a little while but when all is done the terminal should display that 100% data transfer has been reached and all was completed successfully.
- 4) Now restart the website and it should surely look like Figure 15 above, with two maps available.

### **Summary**

We wish that this Server Setup Manual have told you anything and everything you need to know about how to setup and maintain a SCAN Web app server.

Congratulations on your newly gained knowledge and may it serve you well in your future endeavors. Enjoy!





# Index

AFIR.....	4	Github.....	1, 3, 10, 11, 13, 15
Auth0.....	7, 11, 14	Networks.....	3, 4
Build.....	1, 13, 14	Reaction map.....	4
Chemical reaction.....	3, 4, 5	SSL.....	6, 12, 13
Data.....	3, 4, 5, 11, 15	.env.....	11, 14
Docker.....	6, 13, 14		

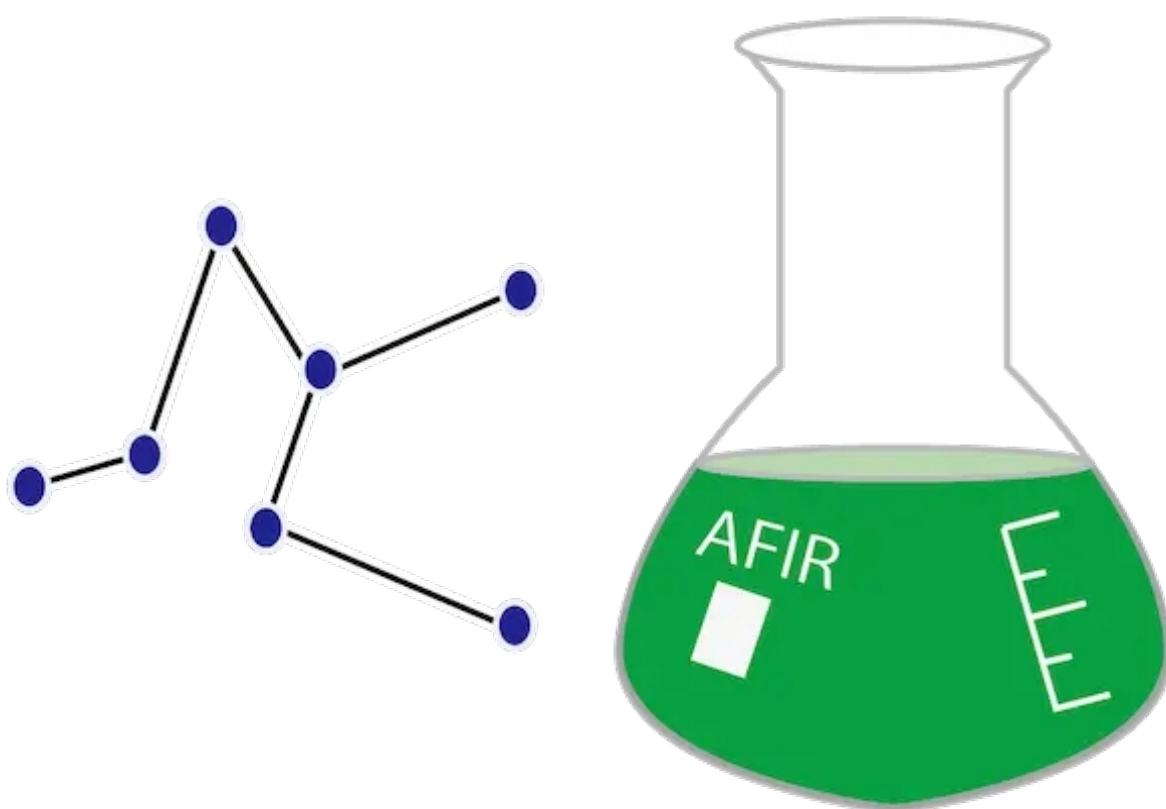
# Figure Index

Figure 1: The front page of the Auth0 website that will be your user accounts manager.....	7
Figure 2: To create a basic User Manager account with Auth0 is free.....	7
Figure 3: The domain name is needed to be obtained before you get here in the process.....	8
Figure 4: In the Auth0 Dashboard you can now configure the login system for your SCAN server..	8
Figure 5: Click yourself to the Default App configuration view.....	9
Figure 6: Scroll down in this view to get to the parts that need to be changed or added.....	9
Figure 7: Make sure you have properly registered the url before this step.....	9
Figure 8: Type in the same url as before, but with the additional path.....	10
Figure 9: Just fill in the same URL as before with no additional paths.....	10
Figure 10: Save the settings and then you are ready to go.....	10
Figure 11: Configuring the .env file in the project root folder correctly is an important part.....	12
Figure 12: Change the names to point at the SSL key location of your computer.....	12
Figure 13: Your local location of the SSL certs.....	13
Figure 14: This is the view you want, showing that the system is all up and running as it should....	14
Figure 15: The SCAN website start page.....	14

# Table Index

Table 1: These are the environment variables that need to be set properly.....	11
Table 2: The SSL certificate keys need to be registered.....	12
Table 3: Make sure you find the correct local location of the SSL certs.....	13

*Thanks for your support*



**SCAN**