TIB Data Manager Manual

(Last update: November 2021)
LDM version 2.3

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1. Description

1.1 About

The TIB Data Manager has been developed to support the aspect of better re-usability of research data.

The prototype supports the management and access to heterogeneous research data publications and assists researchers in the selection of relevant data sets for their respective disciplines.

The prototype currently offers the following functions for the visualization of research data:

- Supports data collections and publications with different formats
- Different views on the same data set (2D and 3D support)
- Visualization of Auto CAD files
- Jupyter Notebook(s) for demonstrating live code
- RDF Description of data collections

The file specific viewers were implemented using CKAN (Comprehensive Knowledge Archive Network) plug-ins to render existing viewers for the datasets included in the CKAN instance.

1.2 Impact on Scientific Data Management

In the research data landscape, there is a high demand for a sustainable and meaningful handling of a main product of scientific work - research data.

Since digital data production has increased rapidly in recent years and an end to this growth is not foreseeable, the availability of these growing volumes of data must be ensured not only for current research but also for future generations. The TIB Data Manager was developed to provide scientists with a **tool to improve the usability of research data**.

The TIB Data Manager provides a data management system that makes it possible to **check the contents of research data sets for their potential application** to the respective domain - **without having to download** them beforehand.

Therefore, the Data Manager enables the visualization of different research data formats and thus supports the **'screening' of data sets** for their potential benefits. As a visualization and management tool, TIB CKAN can be implemented on top of classical research data repositories, which often focus on the (long-term) archiving and publication of research data.

1.3 Application of the Data Manager

As an open source tool, the TIB Data Manager **offers**

● **developers,**
● **scientists and**
● **data curators in public and academic research as well as in industry** a wide range of possibilities for **expanding and connecting established and developing research data management systems** , such as local and discipline-specific research data repositories.

As the German National Library of Science and Technology, we advise universities, research institutions and industry on the use and implementation of the TIB Data Manager. Furthermore, we continue to develop and enhance the functionality of the system in view of the constantly growing number of scientific file formats.

2. How to install

2.1 Dependencies

The TIB Data Manager is composed by different services:

● CKAN: Open-source DMS (data management system) for powering data hubs and data portals
● PostgreSQL: Open-source object-relational database management system
● SOLR: Open-source enterprise search platform
● Postfix: Open-source mail transfer agent (MTA) that routes and delivers electronic mail
● DataPusher:

In order to avoid having to manually install these dependencies, the distribution package comes with dockerized instances of these dependencies, making it easy to get started with TIB Data Manager.

The distribution package also contains a docker-compose file, where
Docker
Docker-compose 1.18.0+

2.2 TIB Data Manager

Docker is necessary so that the TIB Data Manager can be used. To be able to install it, the user must download the docker packets from Docker official website (https://docs.docker.com/install/), and afterwards follow the installation steps established in the packets.

In case the user is going to clone the TIB Data Manager code into your system is also needed to have GIT installed following the instructions in the GIT official website (https://gitforwindows.org).

Note: Before starting the steps below please check that you don't have conflicting docker containers from other projects on your machine. You can check them by firing this command in terminal:

```
docker container ls -aq
```

If you find some of them then please stop them by using the command:

```
docker container stop $(docker container ls -aq)
```

And further after stopping them remove them by the following command:

```
docker container rm $(docker container ls -aq)
```

After doing the steps above continue with the steps below:

To be able use CKAN with all the services it is necessary to follow these steps:

Step 1:

First, it is necessary to change the url of the site in the .env file (which is located in the "docker " folder), in the line 21 of the file the user needs to put the url of the server to get access to the CKAN through the server.

CKAN_SITE_URL : "<URL Server>:5000"

Additionally, make sure the following ports are free in the server:

- Port 5000 for data pusher.
- Port 8000 for Jupyter Notebooks.

Notes:

In **Windows** you can use "netstat" to check whether a port is available.
Use the netstat -anp | find "port number" command to find whether a port is occupied by an another process or not. If it is occupied by an another process, it will show the process id of that process.
For example, in “Command Promt” run:

netstat -ano | find ":5000"

In case the port is free the command shows no results, otherwise if is occupied will show some details like above:

netstat -ano | find ":5000"
TCP 0.0.0.0:5000 0.0.0.0:0 LISTENING 14284
TCP [::]:5000 [::]:0 LISTENING 14284

To check the listening ports and applications on **Linux**:

1. Open a terminal application i.e. shell prompt.
2. **Run any one** of the following command on Linux to see open ports:
   sudo lsof -i -P -n | grep LISTEN
   sudo netstat -tulpn | grep LISTEN
   sudo lsof -i:5000 ## see a specific port such as 5000 ##
   sudo nmap -sTU -O IP-address-Here
3. For the latest version of Linux use the ss command. For example**, ss -tulw**

Step 2:

Note:
If you have knowledge about HTML and CSS and are very sure you are not going to break the source code you can now see the chapter “3. Customizing the Data Manager” before continue for avoiding rework later.

Build the container base of CKAN inside the docker folder.

Inside “Command Prompt” or “Terminal” depending of your Operating System, go to the “docker” folder using “cd” command. For example:

```
cd docker
```

and then run the command:

```
docker-compose up –d --build
```

and then you need to restart the containers to take ckan configuration:

```
docker restart solr db
```

Wait for a minute for letting docker run some tasks in the background and run:

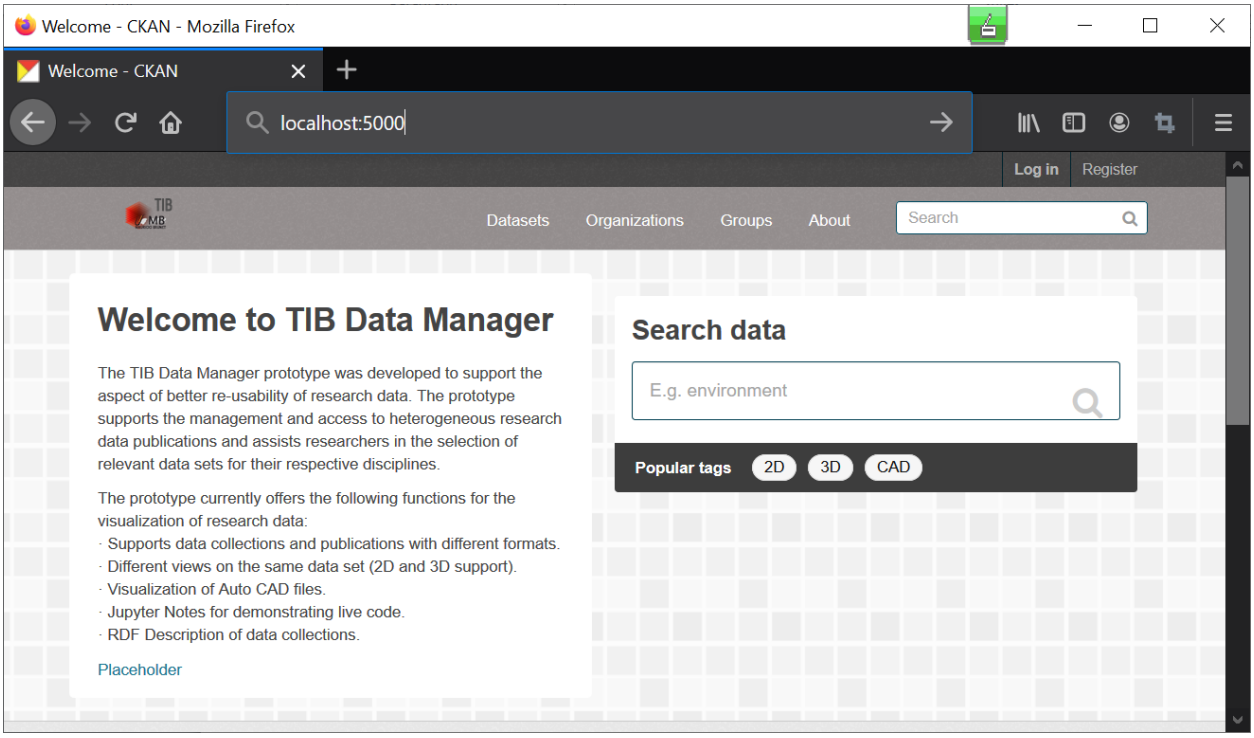
```
docker restart ckan
```

For running the Data Manager in further occasions you can run:

```
docker-compose up ckan
```

Note: Please be patient the dependencies take some time to download.

To open the data manager you must open a browser and enter localhost:5000 or the url that was used in the port 5000.



Step 3:

In case the examples datasets are not showing in the system you can fix the problem running the following command:

```
docker exec -it ckan /reload_database.sh
```

Otherwise, if you need to clean the database and erase all the datasets and TIB examples you can run:

```
docker exec -it ckan /clean_database.sh
```

Troubleshooting:

- "No such file or directory" or other unexpected errors:

Docker outputs all build steps when creating an image based on a Dockerfile. On **Windows systems** is possible to the "exec user process caused **„no such file or directory"**" issue occurred when executing a shell script or many others **unexpected errors**.
The error message is misleading in terms of a wrong file path or path reference. In our case, the issue occurred due to a Windows-style file ending.
We created the Dockerfile on a Windows machine. Saving the Dockerfile used the default Windows file format. This caused the Docker build to fail on a Linux machine.
We fix this converting the file format to UNIX style using dos2unix:
dos2unix your-file.sh
You can run the dos2unix command on any Linux system. If you don't have access to a Linux system, you may use the Git Bash for Windows which comes with a dos2unix.exe.
"Git for Windows" (https://gitforwindows.org/) provides a BASH emulation used to run Git from the command line. *NIX users should feel right at home, as the BASH emulation behaves just like the "git" command in LINUX and UNIX environments.
If you already installed GIT following this manual you are able to open the Start menu by clicking on the Windows icon and typing "Git Bash" into the search bar. The icon for Git Bash and the words "Git Bash Desktop App" will appear. Click on the icon or the words "Git Bash Desktop App" to open Git Bash. Be sure to navigate to the project folder and run the following command:

find . -type f -print0 | xargs -0 dos2unix
This will recursively find all files inside current directory and call for these files dos2unix command

- SERVER ERROR in CKAN's home page:

This could happen if any problem during the installation causes the Databases not building properly.
Try going into a shell inside the ckan container and rebuild the Databases executing the following commands:
docker run --rm -it --entrypoint=/bin/bash ckan

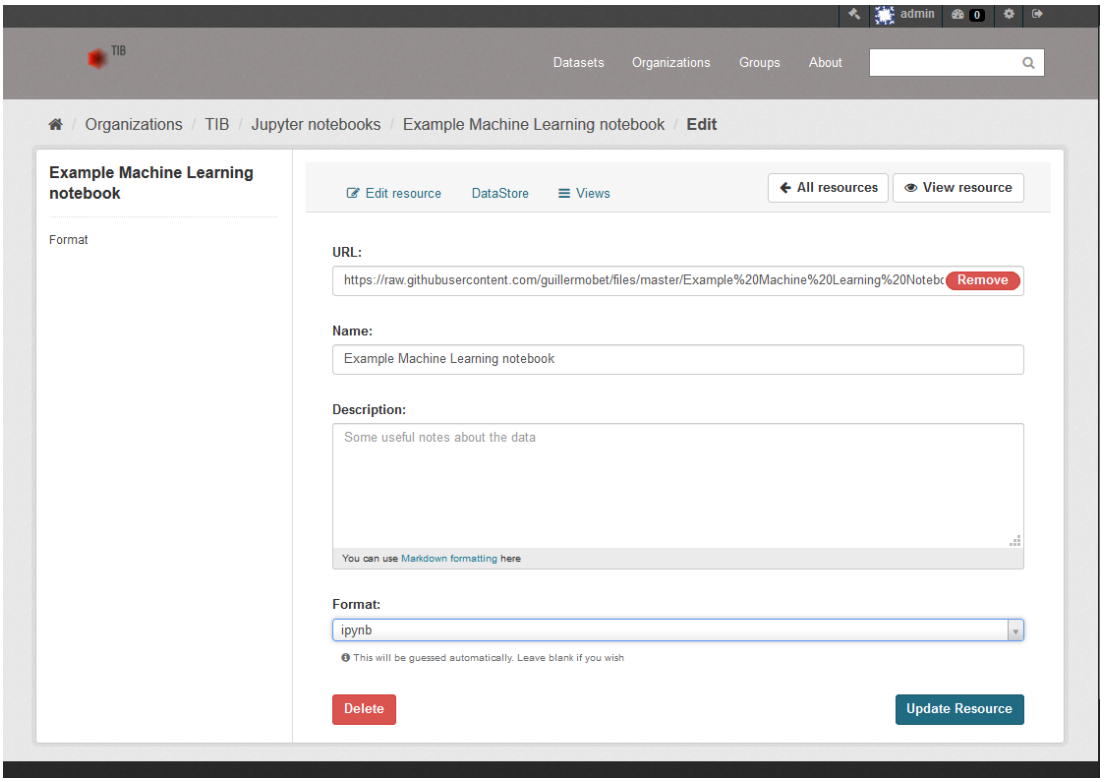
cd /usr/lib/ckan/default/src/ckan

ckan -c /etc/ckan/default/ckan.ini db init

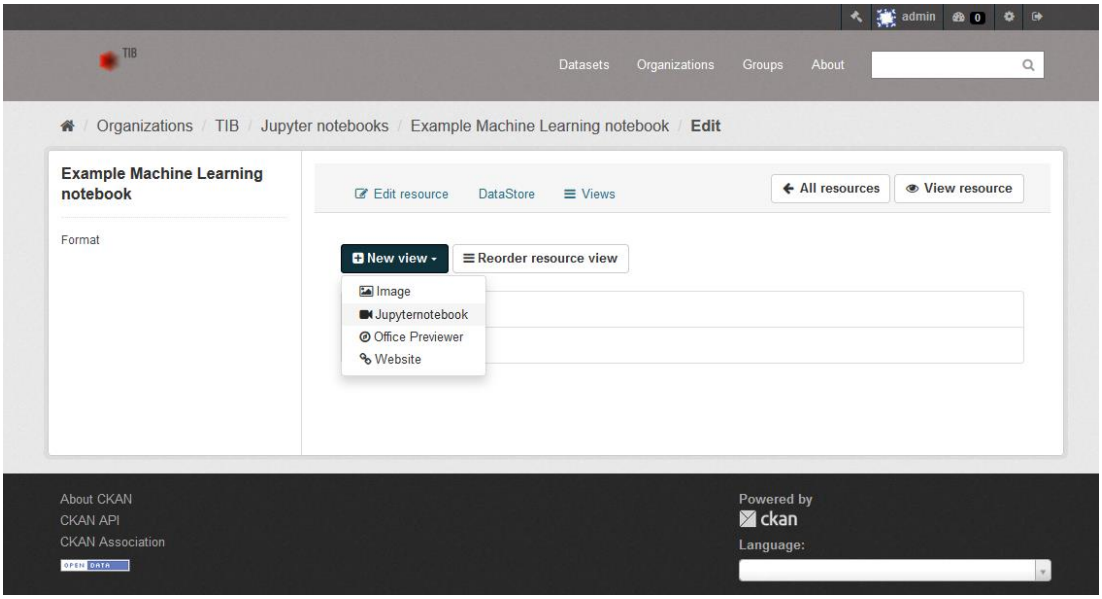
And create admin user with:
ckan-paster --plugin=ckan sysadmin -c $CKAN_CONFIG/ckan.ini add admin email=admin@email.com password=admin

2.3 Jupyter Notebooks visualization plugin.

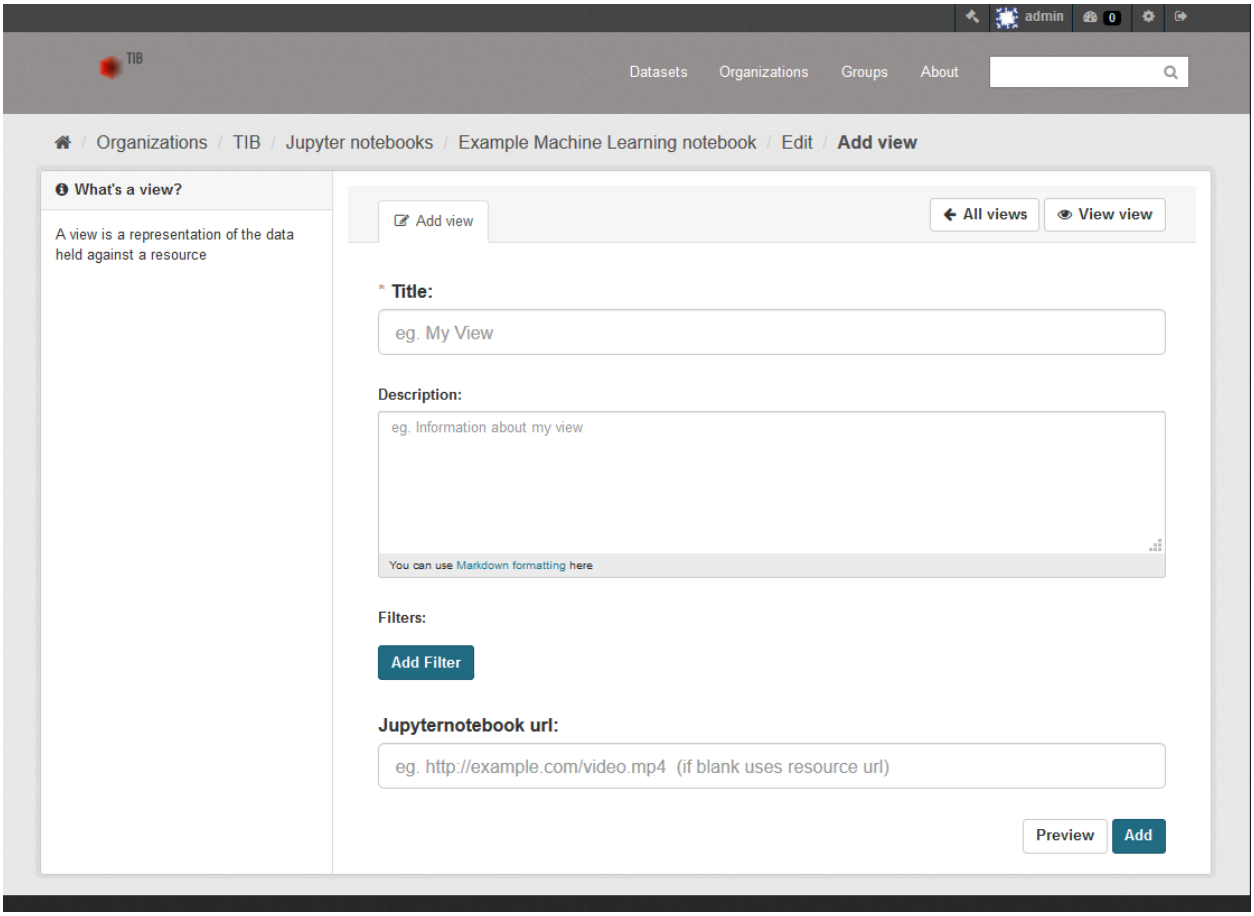
You can view Jupyter Notebooks files using the visualization plugin installed with LDM. For that make sure your notebooks files are described like “ipybn” as format in your resource’s administration page. For example:



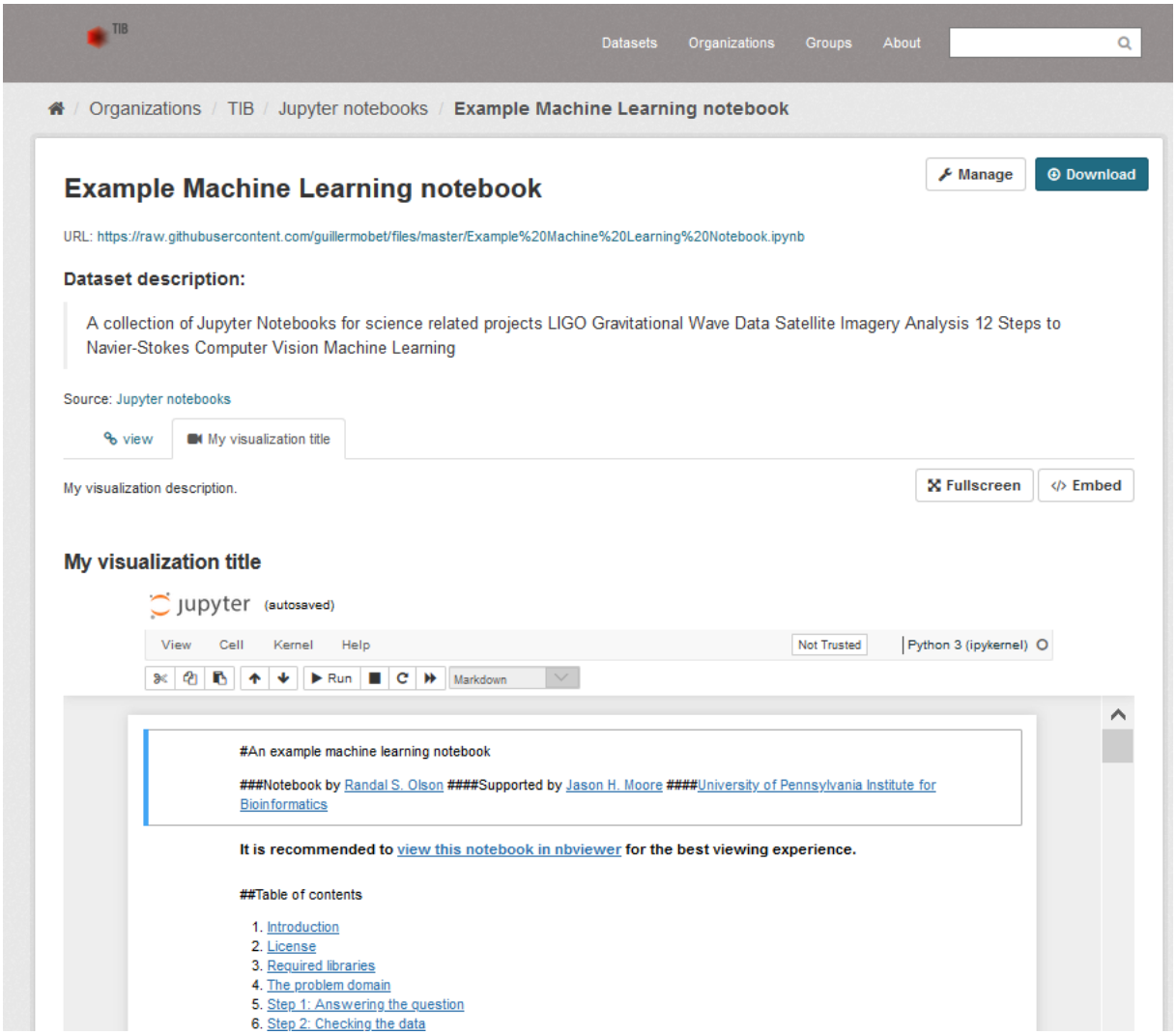
Then you can add the “JupyterNotebook” visualization in the “Views” tab clicking in the “New view” button:



Next add a title and description for your visualization. And in case the visualization should use a different notebook file than the resource itself you can set an URL in the “Jupyternotebook url” field.



Then click “Add” and your view will be ready to be shown in your resource landing page. For example: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Example Machine Learning notebook
Manage
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URL: https://raw.githubusercontent.com/guillermobet/files/master/Example%20Machine%20Learning%20Notebook.ipynb
Dataset description:
A collection of Jupyter Notebooks for science related projects LIGO Gravitational Wave Data Satellite Imagery Analysis 12 Steps to Navier-Stokes Computer Vision Machine Learning
Source: Jupyter notebooks
view
My visualization title
My visualization description.
Fullscreen
Embed
My visualization title
jupyter (autosaved)
View Cell Kernel Help
Not Trusted
Python 3 (ipykernel)
Run
Markdown
#An example machine learning notebook
###Notebook by Randal S. Olson ####Supported by Jason H. Moore ####University of Pennsylvania Institute for Bioinformatics
It is recommended to view this notebook in nbviewer for the best viewing experience.
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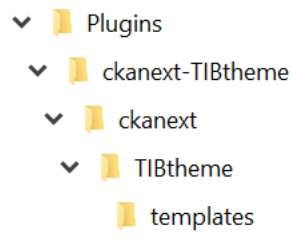
3. Customizing The Data Manager

3.1 Changing The Data Manager Logo

To be able to change the logo of the header of the Data Manager, the user must modify or create the header.html file following the path inside the source files (.\Plugins\ckanext-TIBtheme\ckanext\TIBtheme\templates\header.html):



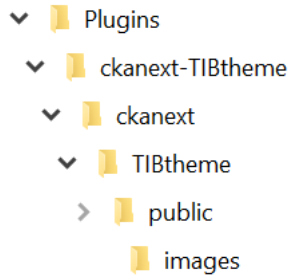
File “header.html”:

```
{% ckan_extends %}

{% block header_logo %}
        {% set url = h.url_for('home') %}
         
         
         
         
        <a href="{{ url }}" style="text-decoration: none;">
         
        <img src="/images/TIB_logo.png" style="margin-top:10px;max-width:30%" alt="TIB" title="TIB">
        </a>
{% endblock %}

{% block header_site_search %}
  <form class="section site-search simple-input" action="{% url_for controller='package', action='search' %}"
method="get">
    <div class="field">
      <label for="field-sitewide-search">{% block header_site_search_label %}{{ _('Search Datasets') }}{%
endblock %}</label>
      <input id="field-sitewide-search" type="text" name="q" placeholder="{{ _('Search') }}" />
      <button class="btn-search" type="submit" style="top:16px"><i class="fa fa-search"></i></button>
    </div>
  </form>
{% endblock %}
```

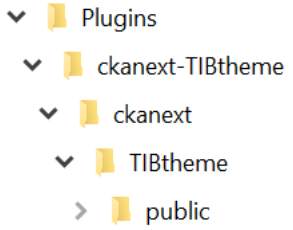
Change the file name “TIB_logo.png” for your custom file name and make sure the file with the exact same name and extension is available in “.\Plugins\ckanext-TIBtheme\ckanext\TIBtheme\public\images\” folder.



For the changes to take effect you need to run again all the installation process (2.2 chapter in this manual).

3.2 Changing The Data Manager Header Color

To be able to change the color of the header of the Data Manager, head to the extensions directory and modify or create a new CSS file in the public directory (.\Plugins\ckanext-TIBtheme\ckanext\TIBtheme\public).
For example create “example_theme.css”.

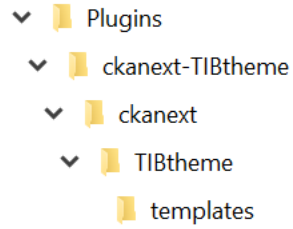


Add this CSS into the **example_theme.css** file, to change the color of Data Manager header:

```
.account-masthead {
  background-color : rgb(40 , 40 , 40);
}
```

*Adjust the values to obtain the desired color.

To make the Data Manager use the custom CSS it is necessary to override the base.html template, this is the base template which the templates for all Data Manager pages extend, so if we include a CSS file in this base template then the file will be included in every page of the Data Manager site. Create or edit the file “.\Plugins\ckanext-TIBtheme\ckanext\TIBtheme\templates**base.html**”



and put this Jinja code in it:

```
{% ckan_extends %}
{% block styles %}
{{ super () }}
<link rel="stylesheet" href="/example_theme.css" />
{% endblock %}
```

For the changes to take effect you need to run again all the installation process (2.2 chapter in this manual).