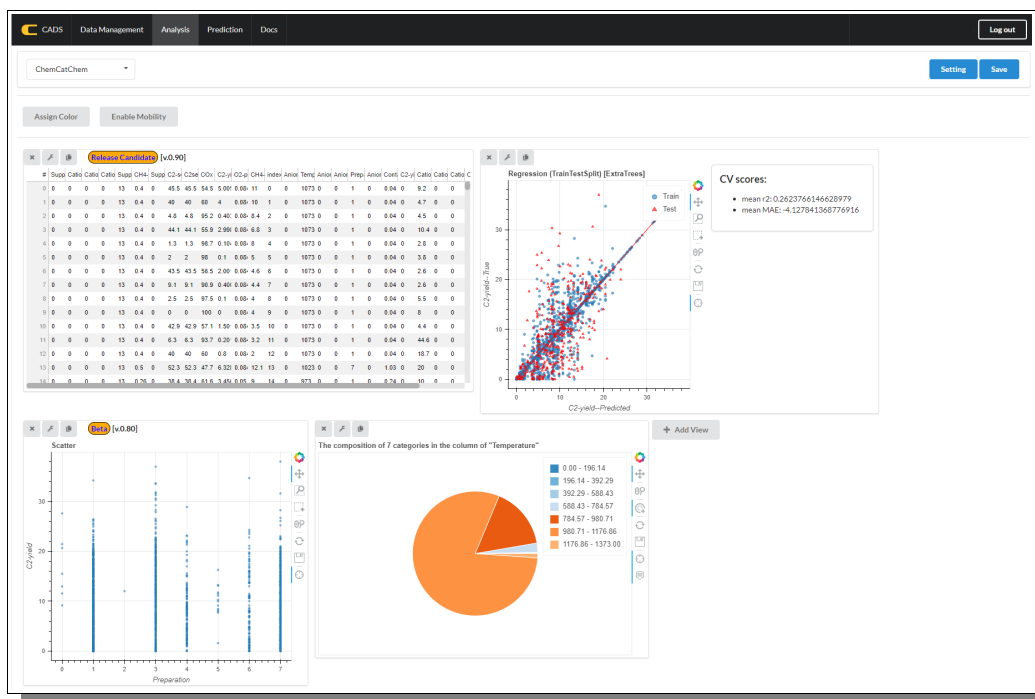
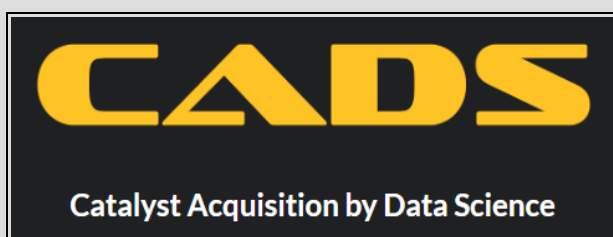


TAKAHASHI GROUP (情報化学研究室)

Hokkaido University



CATALYST ACQUISITION BY DATA SCIENCE



CADS

User Manual

ENGLISH

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Introduction

Get to know what CADS is and what it can do for you as a researcher.

CADS is a catalyst analysis environment that implements a user-friendly graphic user interface(GUI) that aims to help scientist to analyze data in a more simple and effective way without the need of coding and/or setting up complex IT environments.

CADS Overview

CADS provides three basic functions for users: “Data Management”, “Analysis”, and “Prediction”.

Data Management

CADS provides the ability to upload and record individual data as well as data analysis procedures with the option for multi-user sessions, allowing users to share data and analysis reports with collaborators of their choosing. Meaning that not only can a researcher study and analyze their own data, but they can also compare and study other's shared data for a better and deeper understanding.

Analysis

Data visualization tools (scatter plotting, histograms, etc.) and machine learning functions are available for catalyst data analysis and machine learning model selection. This is the core part of the CADS platform and one of its major strengths. In the workspace area a user can load a various buffet of components through which the user can then analyze and manipulate the data for make new findings and getting further understanding. The range of Components is steadily growing and the power of this section is increasing every month. Besides the classic visualization tools mentioned above, there are many more, ranging from image manipulation, machine learning and advanced analyzing and visualization tools, all with simple and straight forward user interfaces that guides the user to do complex analyzing with few and user-friendly operations.

Prediction

Data prediction capabilities are available within the “Analysis” function and inside the Machine Learning components, allowing users to apply and store learning models for predicting new output (e.g. predicting new catalysts). Under the Prediction tab the user can then apply those pre-trained and saved models in order to predict the result with new data.

CADS Architecture

On the surface to the average user the CADS system is just an ordinary website operated by basic mouse

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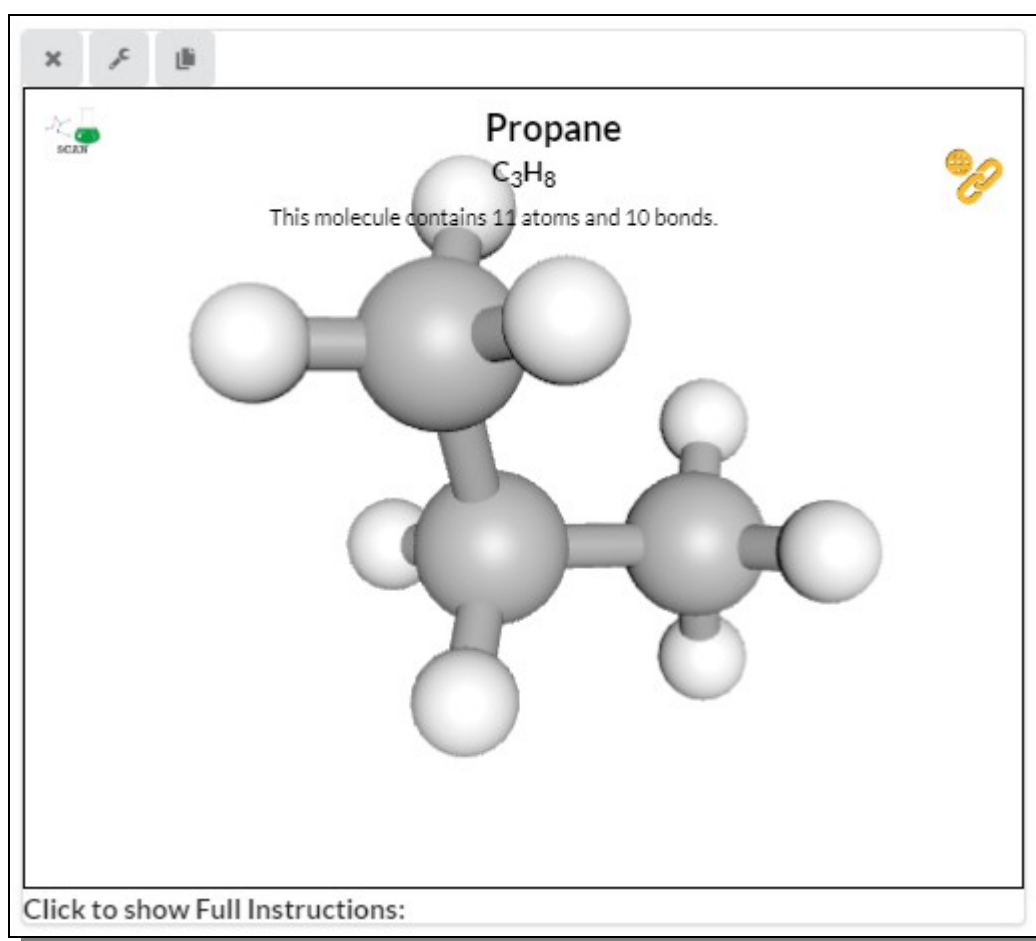
and keyboard operations. A few clicks and perhaps some simple typing of values and then submit to the CADS server, and voila, the data will be displayed in a new graphical and exciting way.

Under the hood the CADS system is built with Django and React JS and for easy maintenance and sound and familiar structure. The custom and generic Analyzing components are using state of the art technology from various high-end libraries for graphical display of data, e.g. Bokeh JS and Plotly JS. On the server side a wide range of support system is feeding the components with all sorts of data management capabilities like SciKit Learn and SciKit Image and much more. This is not needed to be known for the CADS user, but it might be good to know that under the hood are all the well-known complexity the research world is used to, but through CADS, most of the complexity is removed or toned down. Data analyzing should not just be for IT savvy people, it should be available to everyone.

CADS Online in the Browser

In order to use CADS to its fullest one need to have a user account in order to be able to save data and workspaces. Applying for an account is simple and quick and after confirming with a valid email address the CADS system is fully available to use. All interaction from hereon is based on familiar browser interactions using classic form fields and buttons and no need for any plugins or additional downloads are required. All work can be saved and if wanted to, relatively easily shared.

Now, let's go into the details in the next chapter.



User's Manual

So now you sit in front of your computer with the browser open and the CADs website loaded in your current tab. So now what? What should you do and how do you do it? Let's find out together, step by step.

In this chapter We will try to explain everything that you need to know about using CADs in your research and work from a general over-all point of view. Explaining all different areas and what they do and how you interact with it. How you upload your own data and create your own work spaces where you can analyze said data. Details about all the different components will not be shown in this manual, but be found in a component focused manual found on the CADs website. This manual will only focus on general details about all areas and the components.

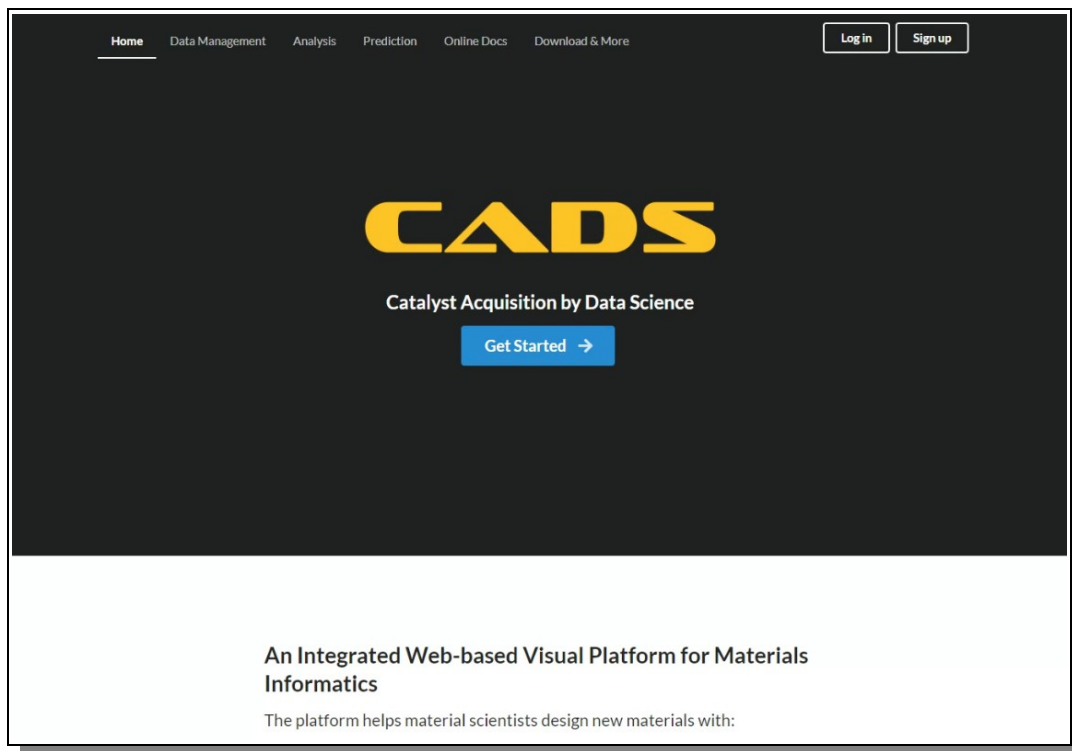


Figure 1: This is the first view that a CADs visitor is met by.

CADS Front Page

The first thing a CADs Web application visitor sees is the CADs Front Page as can be seen in Figure 1. At the top is the main menu that will be visible at all time on all pages as well as the login or logout button

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on the right. If one scroll down to the bottom, one finds is the footer, which is only visible on the front page and not inside the site in general. In the center, middle is the site's short introduction and presentation in texts, images and logos together with a button to "Get Started", which will take the user to Data Management Area explained further on in this document.

CADS Top Menu

CADS's top menu (as seen in Figure 2 below) is how the user navigates between various sections available.

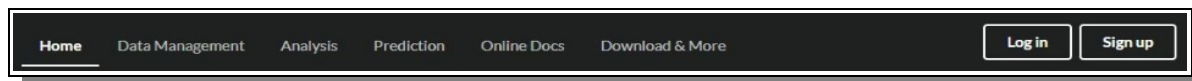


Figure 2: The CADS site navigation menu.

These Sections are 'Data Management' that let us upload and manage data files, 'Analysis' that let us create workspace where one can load various data visualization and manipulation component tools in order to analyze the stored data, 'Prediction' that allows us to get value predictions based on value inputs and pre-saved machine learning models created during the analyzing process, 'Online Docs' which open a simple quick info online manual for those who prefer that and finally 'Download & More' that provides important links related to CADS as well as this manual and more in-depth specialized manuals related to CADS.

To the right side of the top menu the user finds the 'Login' and 'Sign Up' buttons related to the needed user account (explained below).

CADS Front Page Footer

At the bottom of the front page is the CADS footer as can be seen in below.

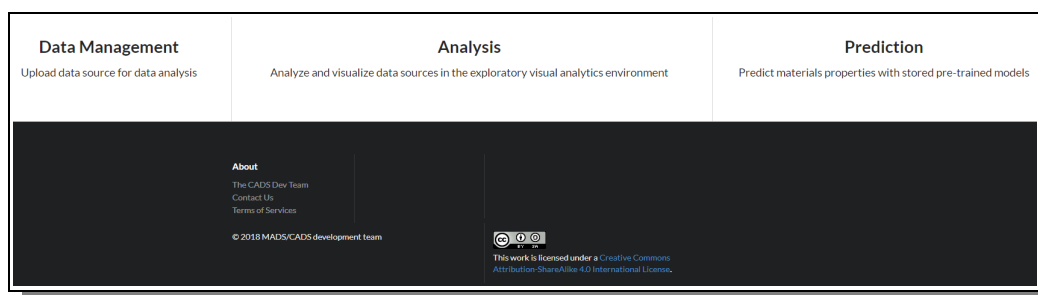


Figure 3: The CADS Front page Footer

Besides some minor information of what CADS is, there are three clickable links. 'The CADS Dev Team' opens the Takahashi research group's website in a new tab which tells you more about the people behind CADS. 'Contact Us' open up a mail link that allows the user to mail the support and the development team with questions and concerns. And the final one 'Terms of Service' explains the legal details in regard of using CADS Online.

CADS Front Page Center

The front page center middle text is just an a small introduction to the site and an invitation to begin using it, mainly by clicking the blue 'Get Started' button that will take the user to the Data Management area. This can be seen in Figure 1.

Sign Up

Before you can use CADS to its fullest, you need to Sign Up and create a user account. If you click the 'Sign Up' button at the top right it will take you to the Sign Up form as seen below in Figure 4.

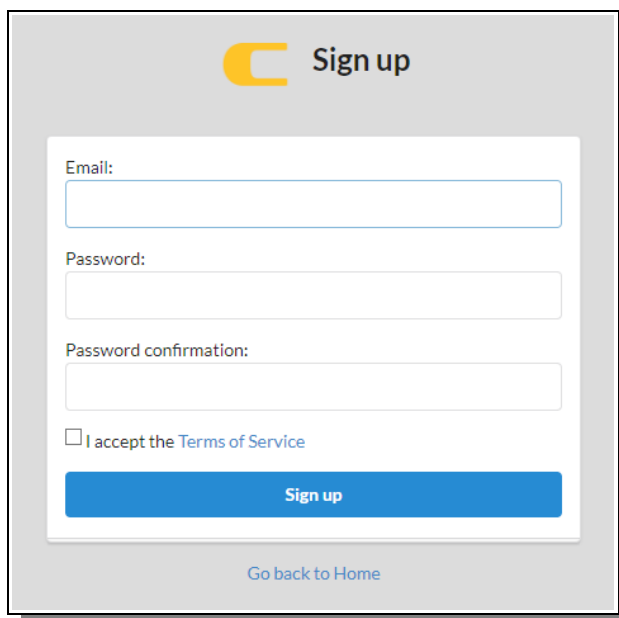
The image shows a 'Sign up' form on a grey background. At the top left is a yellow 'C' logo. The form contains three input fields: 'Email:', 'Password:', and 'Password confirmation:'. Below these is a checkbox labeled 'I accept the Terms of Service'. A blue 'Sign up' button is at the bottom of the form. Below the form is a link that says 'Go back to Home'.

Figure 4: The CADS account Sign Up form

After you properly filled in the form and clicked 'Sign Up' the application will be submitted and an email will be generated and sent to you with an activation link. After clicking that link you will be automatically logged in and forwarded to the CADS start page.

There are some things a guest visitor can do to test the website, but no serious work can be done, including saving, so we recommend to create a user account as soon as possible.

Login

If you already have an account with CADS and you are not yet automatically login as you get to the front page, then you click the 'Login' button on the upper right side as seen in Figure 5.

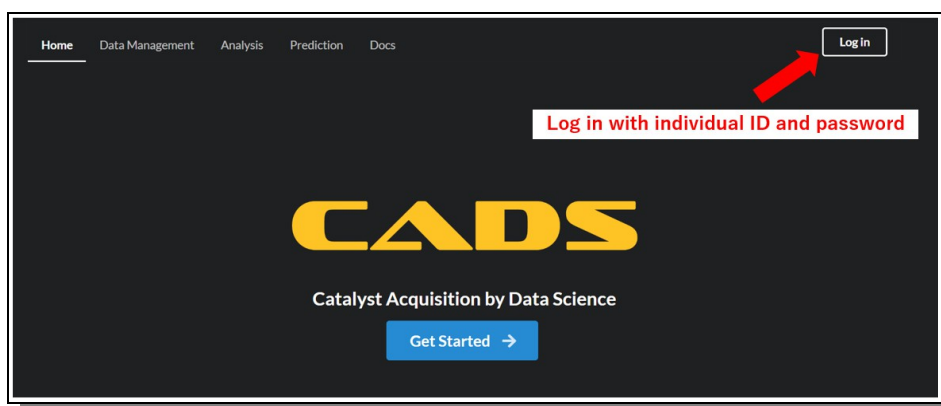


Figure 5: Click the Login Button to login to your CADS account.

When you click there a Login form open up where the user type email and password as seen in below

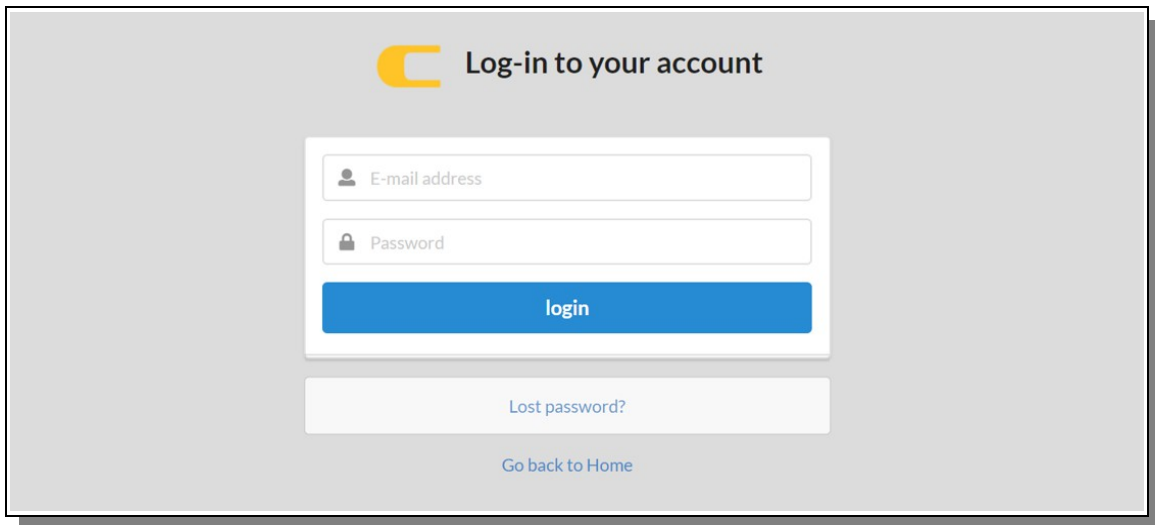


Figure 6: CADS Login form

If one have forgotten the password, you can retrieve it again by clicking 'Lost Password'. It will then be mailed to the email address you used when creating the account. Instead of the Login button the accounts email is now displayed instead.

After you logged in you will be taken back to the front page of CADS where you can navigate to any other page on the site you wish to visit.

Log Out

If you just close the web site without logging out, you will be logged in automatically next time you return within a reasonable time, but if you wish to be properly logged out, just click that button in the top right corner as seen in Figure 7.



Figure 7: The logged in user email and the log out button of the top menu.

Data Management

CADS provides a data analysis environment that can be used with data uploaded into your account. Data uploading is available in the submenu “Data Management” that appears at the top menu bar. In the “Data Management” window, data that is available to your account will appear, including both “public” data and “shared” data. To upload data to your account, click “Add Data Source” on the upper right corner of the submenu bar. This view described above can be seen in Figure 8 below.

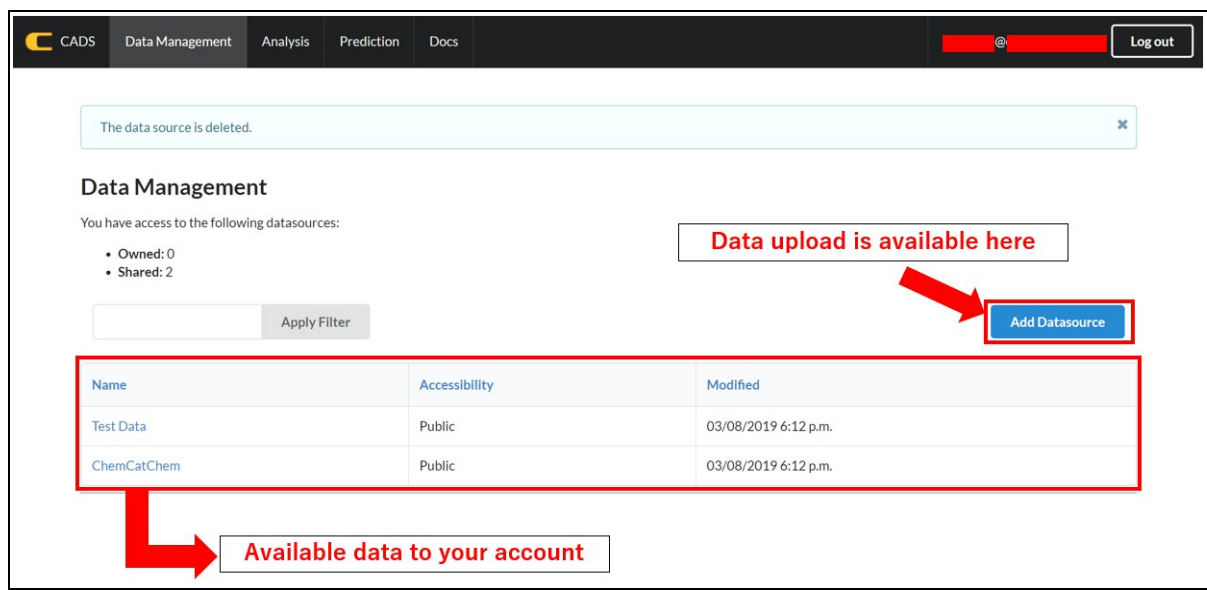


Figure 8: The Data Management front page

Add Data Source

If the user clicks 'Add Data Source' a new view opens up as can be seen in Figure 9 below.

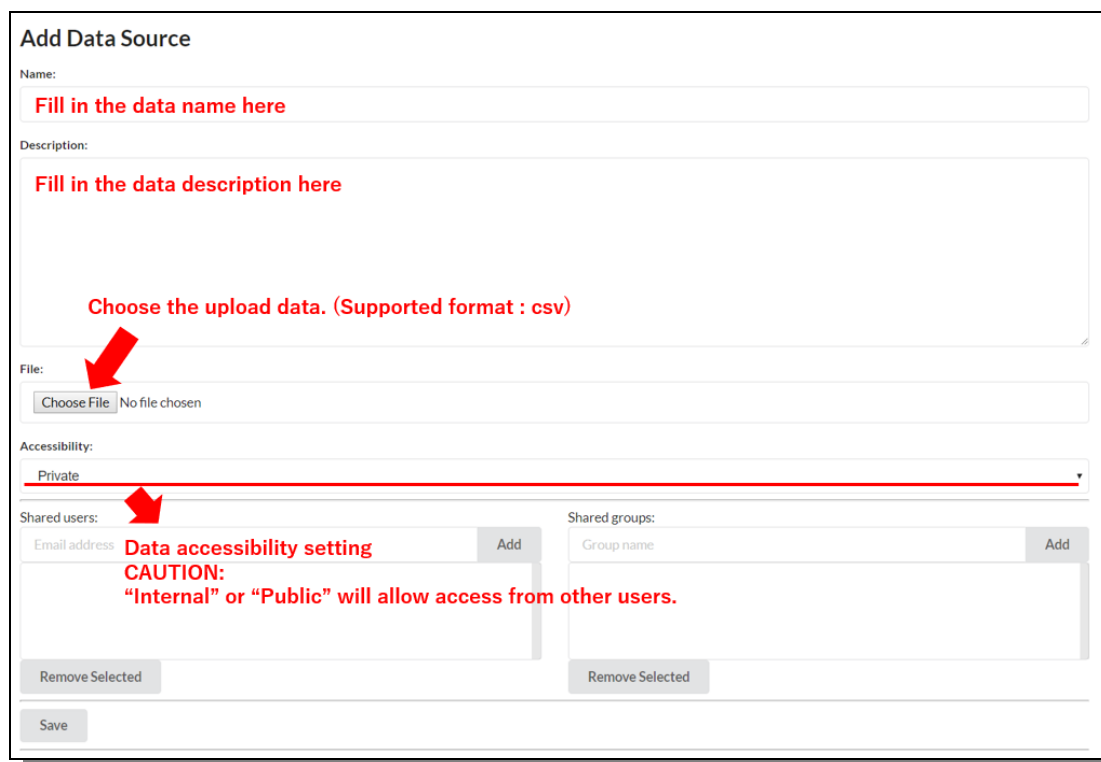


Figure 9: The Add data Source Form

You give the data a name (mandatory) and if you wish also a description (optional), but most important is of course to upload the data itself, which needs to be in CSV-format.

Accessibility is set to private by default, but can also be set to public for all users availability or internal for shared availability where specific users or groups that can access the data is set at the bottom of the

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form as can be seen in Figure 9 above.

When all is filled in as wanted the user clicks Save and is sent to the Data View page where the uploaded data can be viewed. In the Data Management front page the new data will be visible in the full list of available data.

Data View

If the user clicks on any of the available data rows in the list of the Data Management front page, they will be transported to the Data View page where the selected data will be shown as a table with rows and columns as indicated in Figure 10 below.

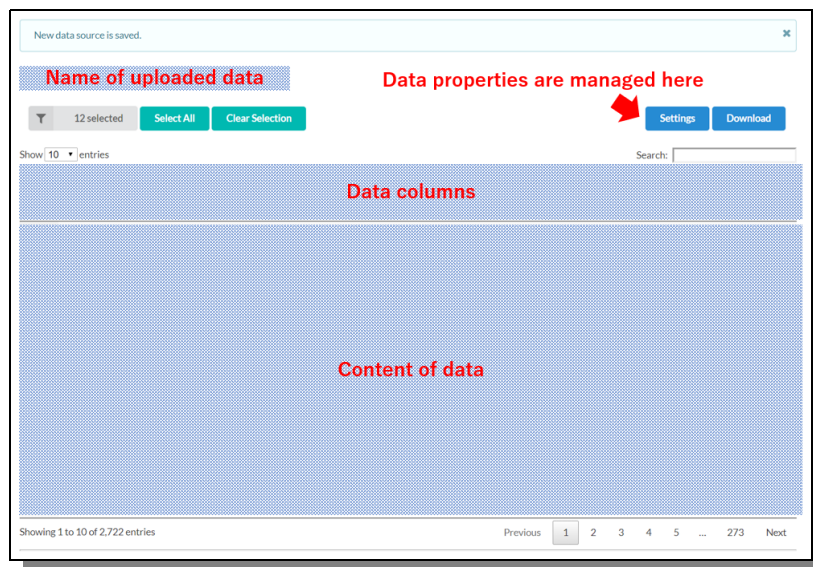


Figure 10: The Data View page with a data table.

To edit the data, one clicks the 'Settings' button in the upper right part of the Data View page, which takes the user to the Settings page as can be seen in Figure 11.

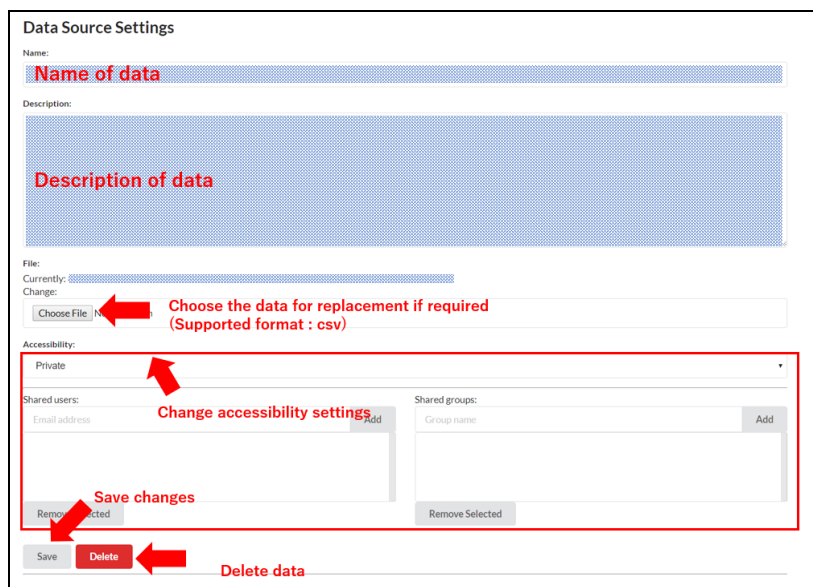


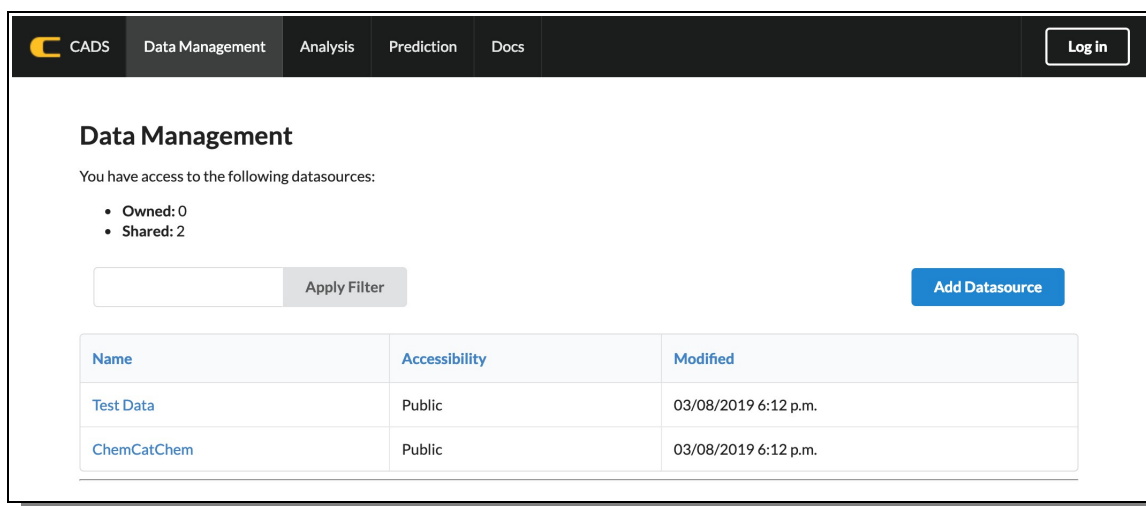
Figure 11: The Data Settings page for changing or deleting data.

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Inside the settings page the user can change most values available at the creation process, including the data file itself, so basically full freedom to update the data if needed. There is also a button for deleting the data post completely. If the "Settings" button is not shown or enabled, it means the data is not owned by you, you only have access to view or use it.

Available Public Data

On the front page of CADS there is one publicly shared dataset available to all called 'ChemCatChem'. As can be seen below in Figure 12. This data set is available for anyone who does not have their own data or just quickly want to try out the website without the need to first upload your own data.



The screenshot shows the CADS Data Management interface. At the top, there is a navigation bar with tabs for CADS, Data Management, Analysis, Prediction, and Docs, along with a Log in button. The main content area is titled "Data Management" and states "You have access to the following datasources:". Below this, there are two bullet points: "Owned: 0" and "Shared: 2". There is a search input field with an "Apply Filter" button and an "Add Datasource" button. A table lists the available datasets:

Name	Accessibility	Modified
Test Data	Public	03/08/2019 6:12 p.m.
ChemCatChem	Public	03/08/2019 6:12 p.m.

Figure 12: The front page of Data Management lists all available data sets, and 'ChemCatChem' is available to all.

If you are interested to play around with the 'ChemCatChem' dataset, below is a shallow explanation of what the data is about.

The 'ChemCatChem' data consists of experimental catalyst data of Oxidation methane coupling(OCM) reactions provided by Zavyalova, Ulyana, et al. "Statistical analysis of past catalytic data on oxidative methane coupling for new insights into the composition of high-performance catalysts." ChemCatChem 3.12 (2011): 1935-1947.

Brief Category Explanations

- *Cation 1–4: Cation composition of catalysts*
- *Cation 1–4: Mol (in molar fractions)*
- *Anion 1–2: Anion composition of catalysts excluding oxygen in molar fractions*
- *Anion 1–2: Mol (in molar fractions)*
- *Support 1, 2: Cation composition of supports*
- *Support 1, 2: Mol (in molar fractions)*
- *Atomic number is assigned for Cation, Anion, and Support.*
- *Preparation – Sample Preparation method*
 - *Numbers are assigned according to the methods listed below:*
 0. *(no data)*
 1. *Impregnation*
 2. *Mech. Mixing*
 3. *N/A.*
 4. *Precipitation*

5. *Pyrolysis*
6. *Sol-gel*
7. *Therm.decomp.*

- *Temperature: Operating temperature in K*
- *p(CH4) and p(O2): Partial pressures of methane and O2 in bar*
- *Contact time: Relation between catalyst bed volume and volumetric flow in seconds*
- *CH4 Conversion %: Methane conversion in mole percentages*
- *C2 Selectivity: Selectivity to ethane and ethylene in mole percentages*
- *COx: Selectivity to CO and CO2 in mole percentages*
- *C2 Yield: Ethane and Ethylene yield – methane conversion · selectivity to Ethane and Ethylene, in mole percentages*
- *C2 Yield Class: Ethane and Ethylene yield in 3 classes, (0:0%-10%,1:10%-20%,2:20%-30%,3:30%+)*

Below in Figure 13 you can see how the dataset is displayed inside CADS Data Management View.

ChemCatChem

Test data for the monitoring test. Data Source Zavvalova, Ulyana, et al. "Statistical analysis of past catalytic data on oxidative methane coupling for new insights into the composition of high-performance catalysts." ChemCatChem 3.12 (2011): 1935-1947. 1864 experimental data

27 selected **Select All** **Clear Selection** **Download**

Show 10 entries Search:

index	Preparation	Temperature	CH4-pressure	O2-pressure	Contact-times	Cation1	Cation1-mol	Cation2	Cation2-mol	Cation3	Cation3-mol
0	1	1073	0.4	0.084	0.04	25	9.2	0	0	0	0
1	1	1073	0.4	0.084	0.04	48	4.7	0	0	0	0
2	1	1073	0.4	0.084	0.04	50	4.5	0	0	0	0
3	1	1073	0.4	0.084	0.04	22	10.4	0	0	0	0
4	1	1073	0.4	0.084	0.04	78	2.8	0	0	0	0
5	1	1073	0.4	0.084	0.04	58	3.8	0	0	0	0
6	1	1073	0.4	0.084	0.04	82	2.6	0	0	0	0
7	1	1073	0.4	0.084	0.04	83	2.6	0	0	0	0
8	1	1073	0.4	0.084	0.04	42	5.5	0	0	0	0
9	1	1073	0.4	0.084	0.04	29	8	0	0	0	0

Showing 1 to 10 of 1,866 entries Previous 1 2 3 4 5 ... 187 Next

Figure 13: ChemCatChem dataset as it can be viewed inside CADS Data Management

Analysis

Of course, the main concept of CADS is not to view the data in a simple table, no matter how fun and useful that can be at times. No, the main idea is to analyze and manipulate the data in multiple various ways, to analyze it, with the use of a large range of different components, and by thus, make new discoveries and find new ways in the search of what ever one is searching for. And where better would that not be done than under the 'Analysis' item in the top menu.

Workspaces

The first page one will see when entering the Analysis section are the available workspaces.

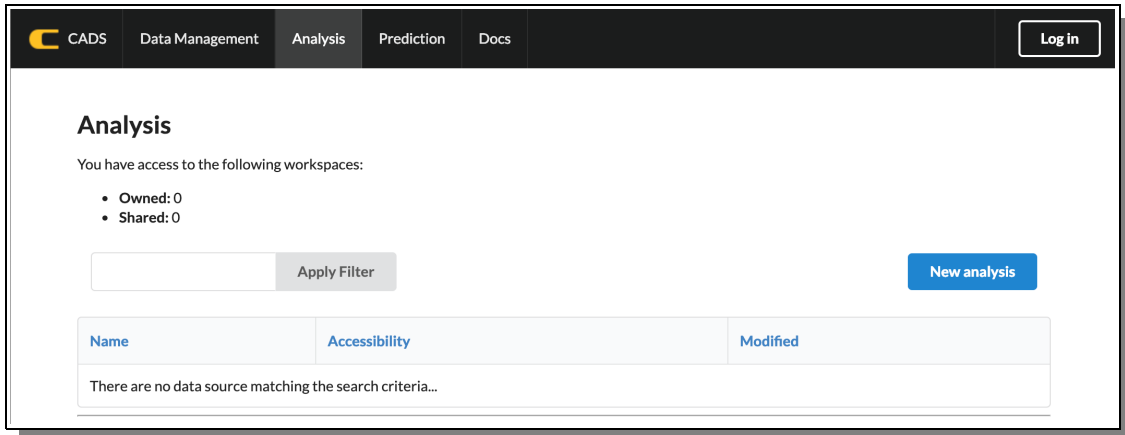


Figure 14: The first page in the Analysis section is the available Workspace list area.

If this is their first time visit, that list is most likely empty, but if another user has shared a workspace with the user then it will also appear here. Figure 14 shows this view.

A workspace is an 'Analysis' setup, using as specific chosen dataset, visualized, configured and modified using a specific range of chosen analysis-components (described further below in general terms and in detail in a separate 'Components Manual'. The number of available workspaces are displayed at the top of the page, above the list itself.

To create a new and fresh workspace, the user clicks the 'New Analysis' button to the left of the page and will then be taken to the analysis workspace area.

Inside the Workspace

Inside the new workspace there are a few buttons to use in order to setup an analyzing area to look as envisioned. Figure 15 Shows how the empty workspace looks like and which buttons are available at start.

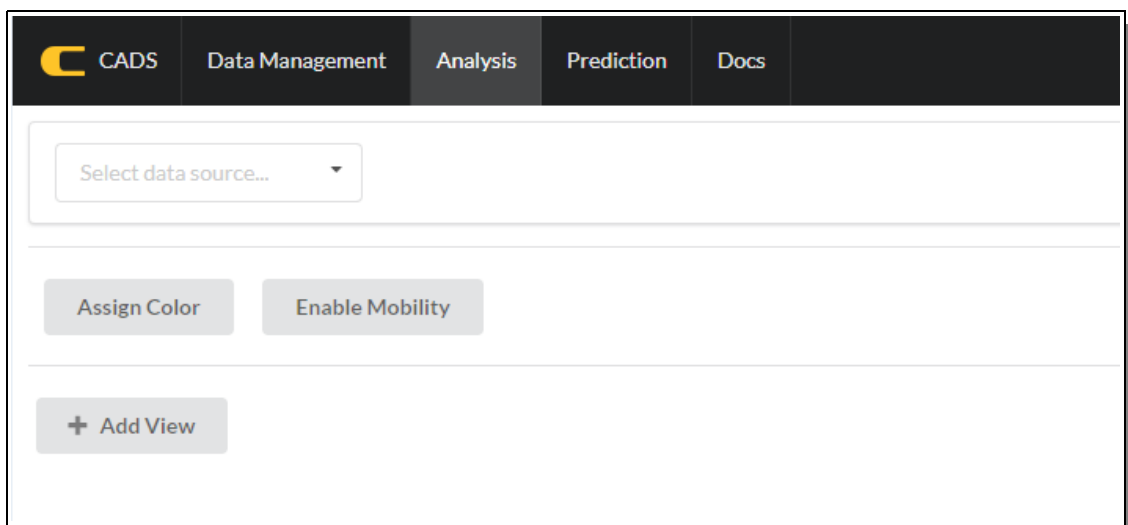


Figure 15: An empty Analysis workspace with no components and no selected dataset.

The first thing to do is to pick which dataset to analyze. The available datasets are the same ones that

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was visible in the Data Management section, and can be selected via a drop-down box in the upper left corner. When selected, all components being loaded in the work surface area will use that dataset, some fully automatically, other after some configuration.

To load a component, the user click on the '+ Add View' button that will open up a small form with a drop-down box where the user can select which component view to insert, as seen in Figure 16.

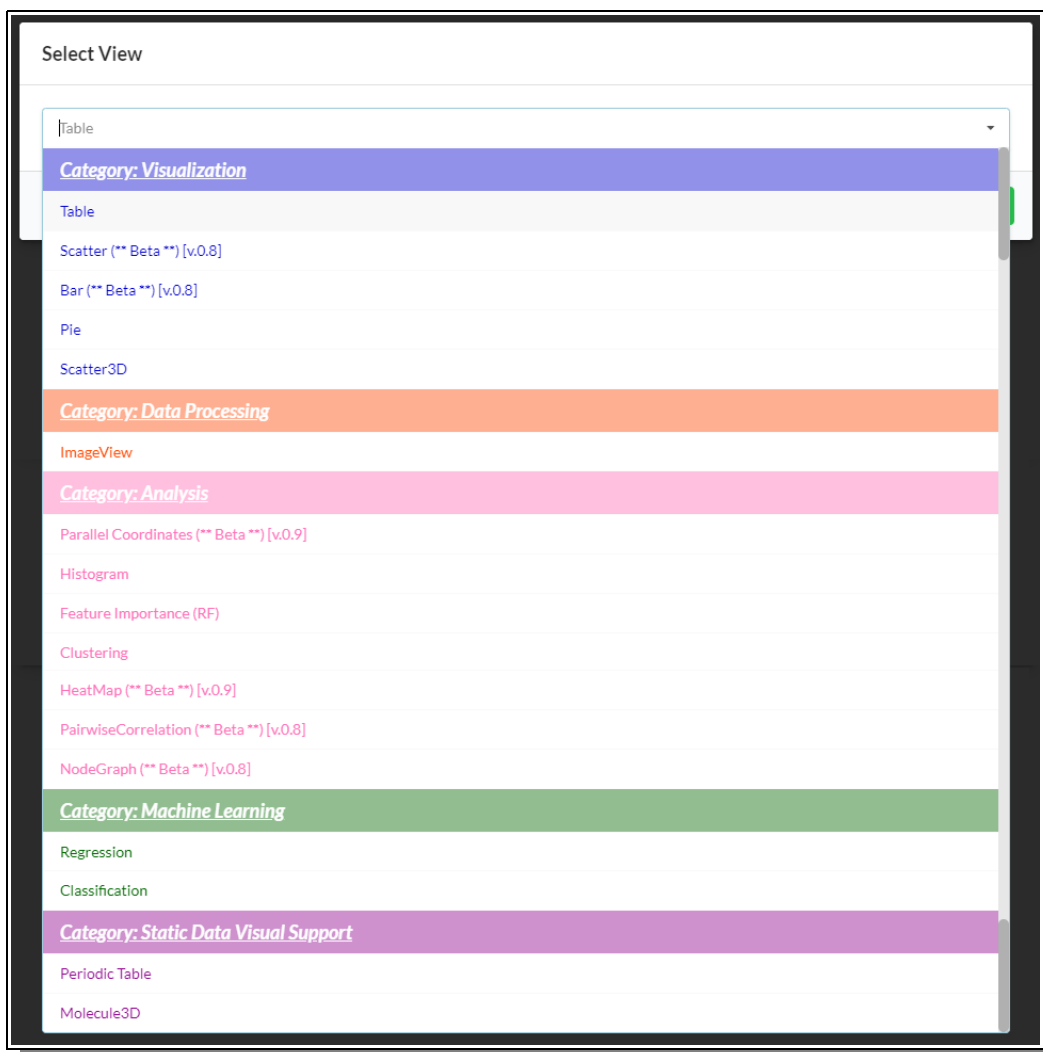


Figure 16: These are the components available in May 2023, but there are always more being added.

The amount of components available are constantly increasing, and details of what each component do and how to configure them can be found in the dedicated Components Manual, found on the CADS website.

View Components currently comes in five different categories; Visualization, Data Processing, Analysis, Machine Learning and Static Data Visual Support. None of these categories are chiseled in stone or are clearly defined, and many components could fit inside several categories, but it provide some form of help to the user to find the type of component they are specifically looking for.

After the user selected a View Component and pressed OK, it will be loaded into the workspace. Every new component will be inserted at the end of the range of components, if the order needs to be changed that is no problem as can be seen in the description further on.

In Figure 17 below one can see two components loaded into the analysis workspace connected and

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configured to show some aspect of the dataset that is currently used.

If one would change the dataset, all the currently loaded and displayed components will more or less reset to its initial default state, and has to be reconfigured with the new data.

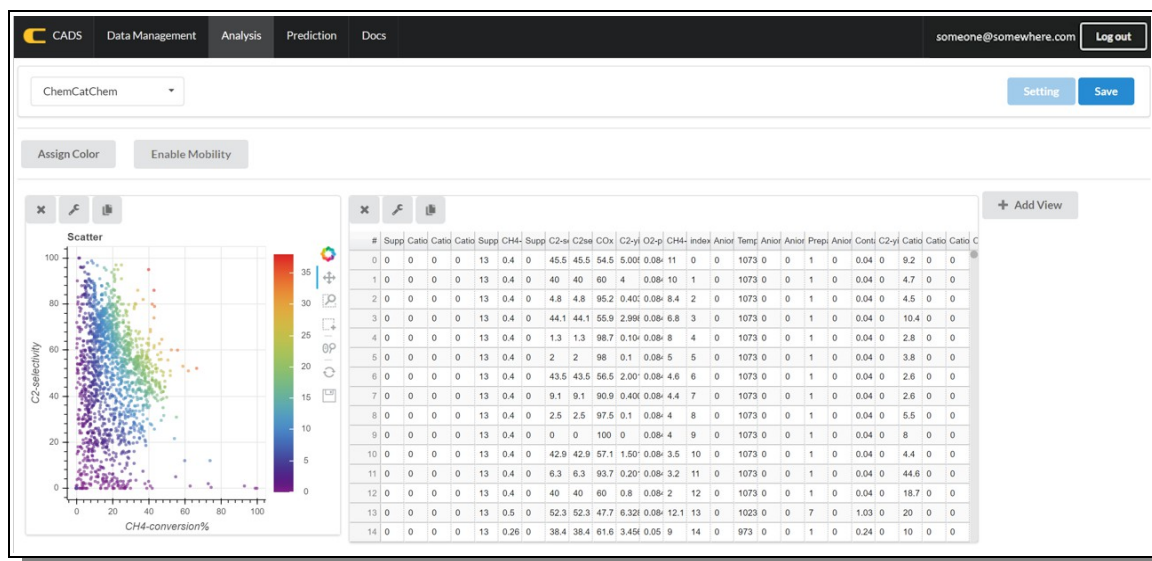


Figure 17: Two different components loaded into the analysis workspace, configured to show the dataset loaded.

There are a few buttons available, both in regard to the workspace itself, but also inside each component. Let's take a closer look at each and understand what they do.

The first button that says 'Assign Color' will do nothing if no subset of data is selected in any of the components, but if there is, a color will be automatically selected for that subset and applied in all present components that deals with data selection and a button representing that color will appear next to the 'Assign Color'-button. Selecting a new subset and click the 'Assign Color' again will assign a new color to that subset, and it will be visible in the components.

If the colors assigned by default is not the color wanted, then the user can change that by clicking on the wrench icon on the color button and make that change as can be seen in Figure 18 below.

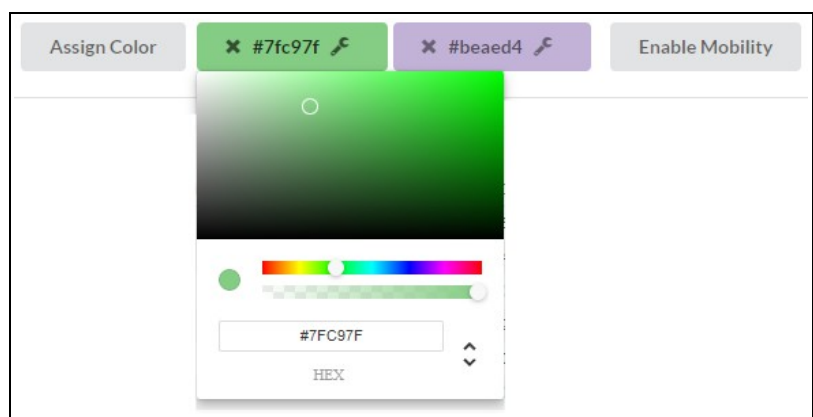


Figure 18: Assigning colors to data subsets is easy and quick.

To delete a color and reset the subset to its original default color in the data visualization, just click the X and the color will disappear.

If the user clicks the 'Enable Mobility' button, it turns green to indicate mobility-mode is turned on. To

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turn it off, just click the green button again, and it switches off and goes gray again. In Mobility-mode a dragging handler button appear in each component that allow the user to move the components around freely in the workspace grid to get them in the order they want. Each component also gets a resize handler at the bottom right corner that allows for easy and quick resizing. In Figure 19 below one can see the Mobility- mode enabled

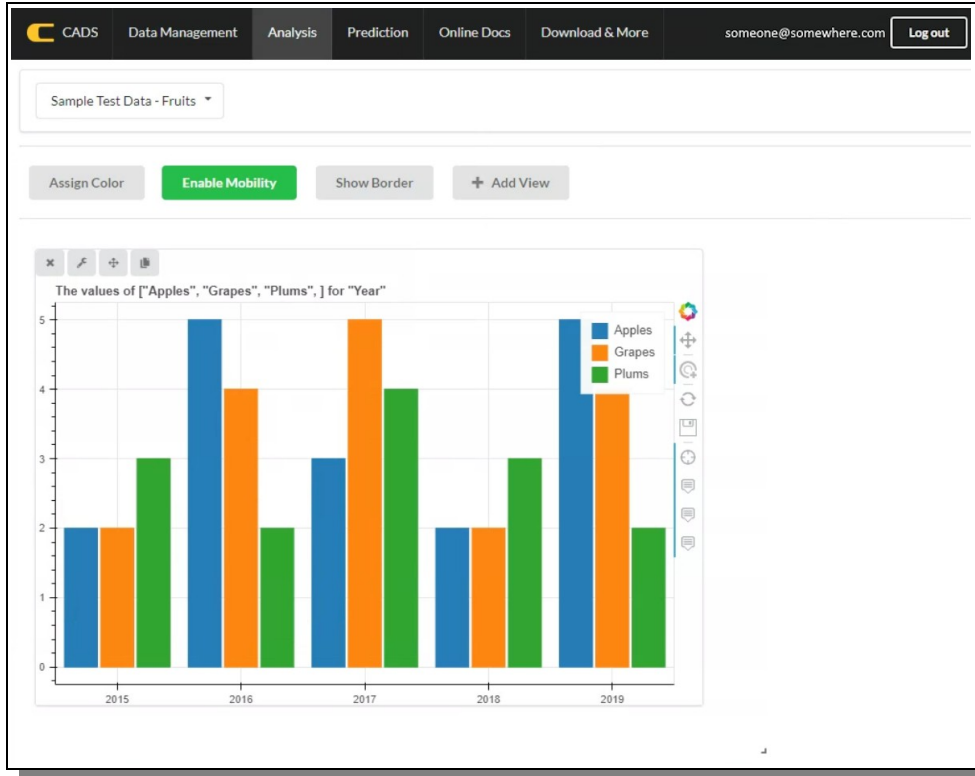


Figure 19: Enable Mobility let the user rearrange and resize components via mouse operations.

By using the mouse and drag the component via the drag handler in the component the user can move it around, and by clicking and moving the resize handler the size can easily change. While moving or resizing the area affected turns pink for visual aid. Below in Figure 20 one can see this in action.

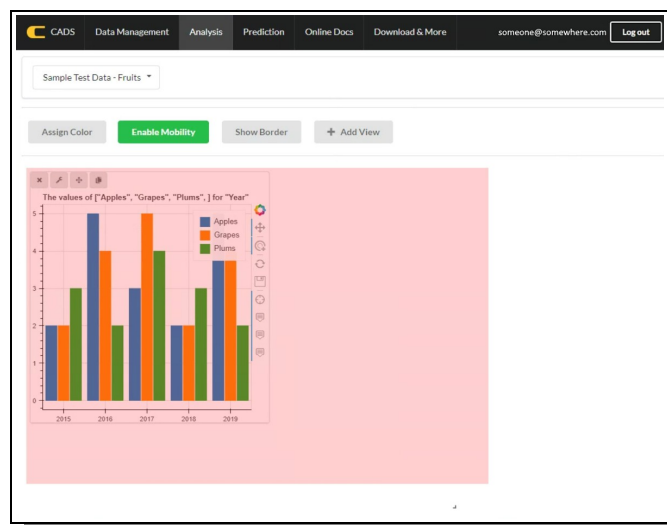


Figure 20: Resizing a component in the workspace

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One can change components size manually via the component form to, by typing exact values, but this an optional way.

Another button that also appears when in Mobility-mode is 'Show Borders'. This button is just for some additional visual aid, and it shows a border around all different parts of the workspace as seen in Figure 21 below. It is usually not needed. Even though one can be in Mobility-mode at all time, it is usual better and smoother to only switch it on while moving and then switch it off again, when finished.

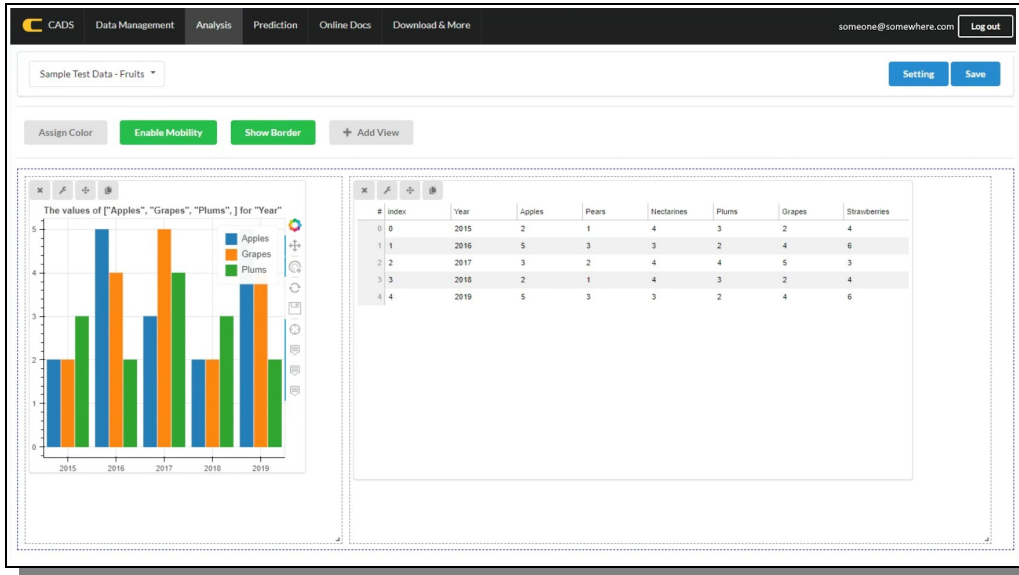


Figure 21: Showing the Workspace and components borders for visual clarification.

In Mobility-mode the '+Add View' button also moves from the workspace itself to the top button area.

In the top right corner there are two blue buttons. The first 'Settings' is disabled if the current workspace is not yet saved, and the second 'Save' button allow the user to save the current workspace with all its current components and their respective configurations for easy access at a later time as well as the possibility to share with others.

When Save is pressed a small form opens that requests the user to give the workspace a name (unique names are not required, but perhaps help the user differentiate between multiple saved workspaces).

If the workspace has already been saved before, then the user have the opportunity to save under a new name or use the previously used name and overwrite the current saving.

A message is displayed after clicking 'Save' that confirms the success of the operation.

The 'Setting' will open up a larger form that allow the user to add additional information but also share the workspace with other CADs users. This form looks and works similar to the Data Setting form described earlier and was shown in Figure 11.

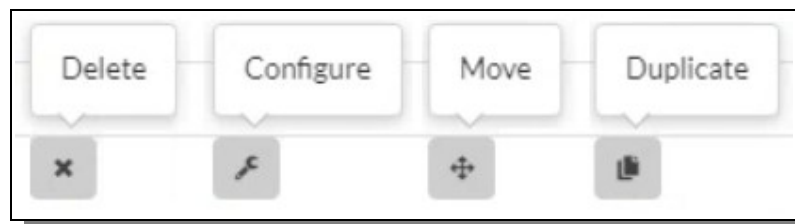


Figure 22: The possible four different buttons available in all components.

When a component is loaded it also comes with its own set of buttons. Both default ones in gray, same

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for all components and four at the most and as can be seen in Figure 22 above , but sometimes also its own unique buttons for that specific component, usually displayed in yellow.

Let's look at the shared default ones and see what they do.

The first button, is the 'Delete' button and it does just that, it deletes the component in question. CADS does not have any regret buttons, so if the component was not saved alongside the workspace, then it will be gone forever after deleted, and has to be recreated from scratch if wanted again.

The second one is the 'Configure' button and it will open a unique configuration form for the specific component that allows the user to configure the component to look and feel and behave a certain way. Below in one can see an example of one of these component configuration forms.

The image shows a configuration form for a bar chart component. The form is titled "Bar [1]". It contains several sections: "Enable Transpose View" with a toggle switch; "Dimension" with a dropdown menu set to "Year"; "Mesures" with three tags: "Apples", "Grapes", and "Plums"; "Filter" with a dropdown menu set to "ColorTags"; "Extent" with two input fields: "Width" (697) and "Height" (450); "Bar Direction" with a dropdown menu set to "Vertical"; "Legend Location" with a dropdown menu set to "top_right"; and "Color Palette" with a dropdown menu set to "Category10 (max 10 colors)" and a color swatch below it. At the bottom right of the form are two buttons: "Cancel" and "Submit".

Figure 23: An example of a configuration form for a component (in this case a bar chart)

Since every configuration form is unique we will not go into any details here, instead you can read about that in the Components Manual found on the CADS website.

The only shared properties though, is that the type of component and its internal ID is shown at the top and at the bottom there is a Cancel and a Submit button. The later is sometimes disabled if certain values are not yet filled in. Most components also share the Extent fields for width and height of the component for manual detailed resizing by numbers.

The third button is the 'Move' button and mobility handler which is only shown if mobility-mode is enabled, otherwise it will be hidden. How to use that is explained above.

The forth and last default button is the 'Duplicate' button that does exactly what it sounds like, create an exact duplicated copy of this component and insert it to the right of the original. An easy and quick

way to add same type of components but avoid redoing a lot of the configurations.

How multiple components can share the same workspace and be combined in highly visual ways is partly up to the imagination and skill of the user, but also something that depends on the individual components and is explained further in the components manual, but for all basic understanding of a workspace and default looks of components you should be ready to go.

Prediction

In some of the Machine Learning components inside the analysis area, like e.g. Regression and/or Classification there is an option to save the training model and use it for predictions after it has been created and trained. In Figure 24 below there is an example how that saving is done, by clicking the 'Save Model' button inside the configuration form and giving it descriptive name.

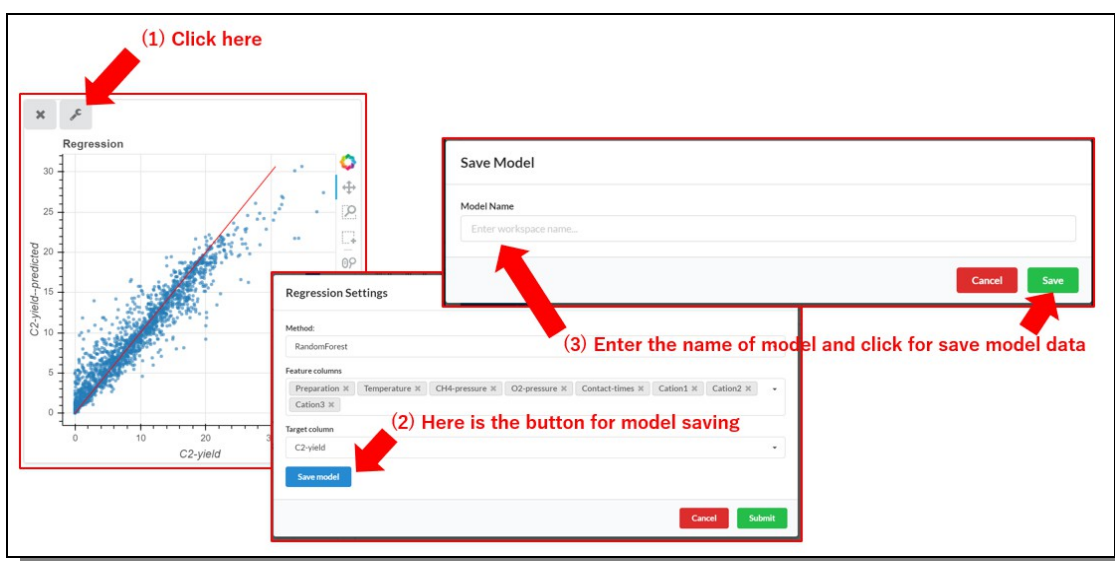


Figure 24: The process of saving a machine learning training model to CADS for later use.

After a model is saved it can be located in the Prediction section found in the top menu as can be seen in Figure 25 below.

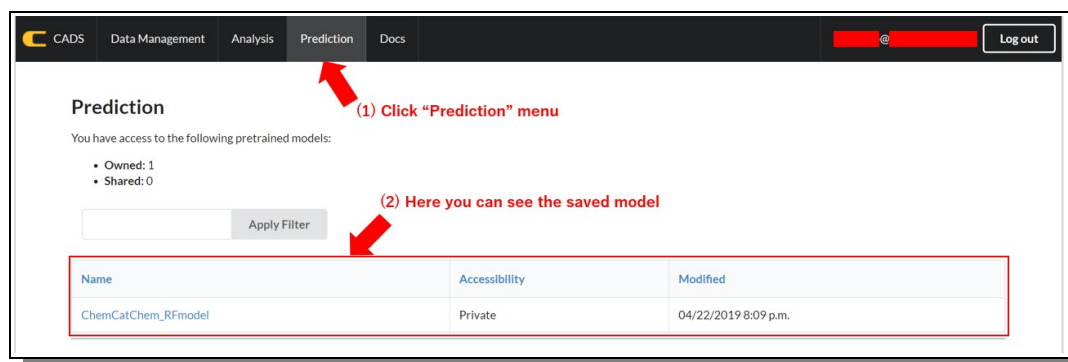


Figure 25: Inside the Prediction section one would find ones saved ML models.

If a model have been previously saved it appears in the list of available models in this section of CADS. To view, edit or use this prediction model, the user just clicks the name and they will be transported there.

Inside the model one has a a set of two familiar buttons at the top right corner, 'Settings' and 'Delete'. 'Delete' do exactly that and completely removes the prediction model from storage and cannot be

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retrieved again. The only way to get it back would be to retrain the component as described above and save again. 'Settings' would take you to a similar page/form like for Workspaces or Datasets as previously seen in Figure 11 , where one can edit and save the description and sharing options of the prediction model.

Besides those buttons, there is the actual prediction interface seen where the user can add values to the parameters available according to the training data. After filling those values in, one can click the 'Predict' button at the bottom and the model will then predict the value for the target column based on the ML model which was created. Below in Figure 26 there is an example of this.

ChemCatChem_RFmodel

Settings Delete

Preparation: 900

Temperature: 0.3

CH4-pressure: 0.5

O2-pressure: 2

Contact-times: 3

Cation1: 7

Cation2: 15

Cation3: 34

Predict

Prediction result

C2-yield: 16.374679999999998

(1) Input the certain feature variables for the prediction

(2) Click for prediction, then the result appears below

Figure 26: Inside a prediction model one can predict target column values.

Online Docs

There are some simple and basic instructions without any major details on how to use CADS in a more quick access way with some useful pointers for anyone that do not wish to go for this or additional manuals at all time. These online instructions are reached by clicking the Online Docs sections in the top menu of CADS which opens up a new tab and load the page that can be seen in Figure 27 below.

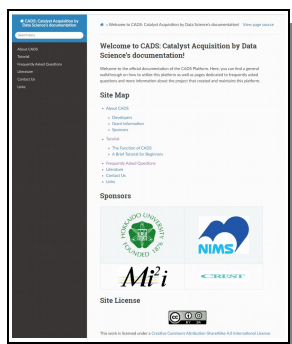


Figure 27: The Online Docs gives some parts of this manual's information in a quick way.

Download & More

Under this section in the top menu one would find this manual and other documents for detailed information on how to use CADS in various ways. There are also some links to external sites and documents that expand on CADS or contains additional information on matters related to CADS and what CADS can do as well as academic papers published in direct or indirect relation to CADS. Below in Figure 28 is an example of how this section usually looks like.

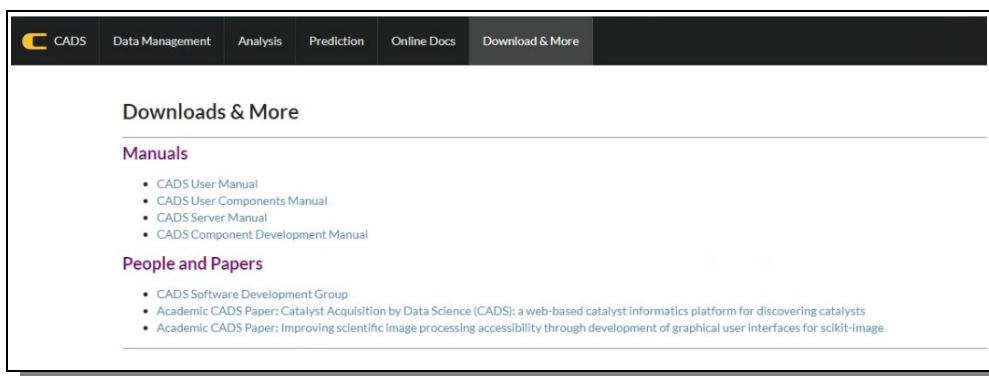


Figure 28: Here one can download CADS manuals and academic papers and more.

Summary

We wish that this manual have told you everything you need to know about CADS Web application from a general point of view and how to use it. Feel free to return here whenever your memory fails you on what to do and when.

Also, please read our other detailed manuals on how to use each individual Analysis components currently available, our manual on how to setup and maintain your own CADS server and/or our development manual on how to code and develop new CADS components.

Congratulations on your newly gained status as a 'CADS-User'. Now it is time to do some serious research. Enjoy!



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