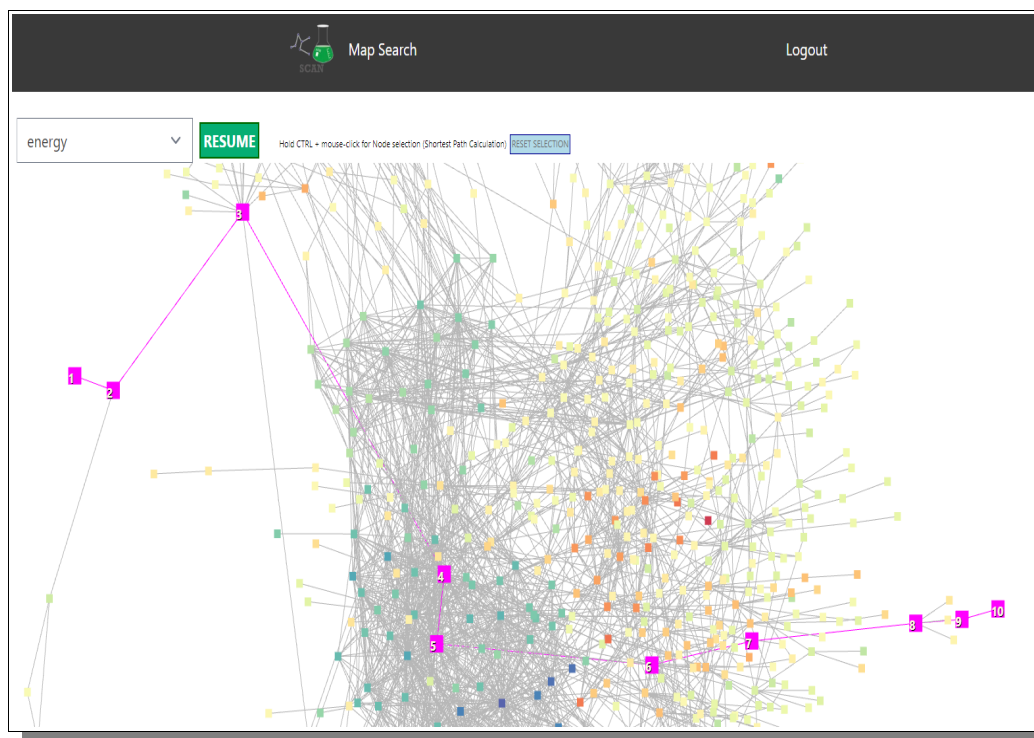


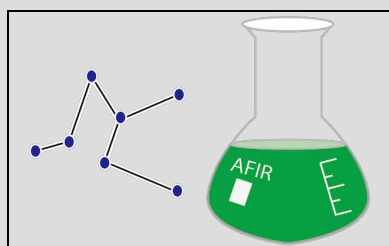


TAKAHASHI GROUP (情報化学研究室)

Hokkaido University



WEB APPLICATION FOR SEARCHING CHEMICAL ACTIONS AND NETWORKS



SCAN

User Manual

ENGLISH ORIGINAL

SCAN User Manual

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SCAN Web Application

[Searching Chemical Actions and Networks]

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in Takahashi Group (情報化学研究室) of Hokkaido University

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For any further information, visit the project GitHub at

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

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Preface

A few words from the creators.

This manual is attempting to be an extensive guide to anyone who wishes to use the SCAN web application found online at <https://scan.sci.hokudai.ac.jp>. 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. Currently there is no option for users to upload personal chemical reaction networks, but instead the users are given the opportunity to load, view and analyze pre-loaded data maps that is currently provided to SCAN by the independent data-team who are cooperating with the SCAN dev team. The data chosen and provided from the data team is a collection of AFIR data (Artificial Force Induced Reaction), that is generated by a research group iReDD at Hokkaido University lead by Professor Satoshi Maeda. From a pure SCAN development team's point of view, there is no limitation on what type of data which could be loaded and analyzed in the application, but for the time being the data team is only providing AFIR data.

So to be clear, the SCAN software development team is not involved in choosing and uploading the currently available 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 or any data available on the site.

For any data related issues, please contact the iReDD (<https://www.icredd.hokudai.ac.jp>) team at Hokkaido University.

If you, when using our software, find any issues or come up with any suggestions for improvement, that is related to the software itself, please feel free to contact us and let us know. SCAN is still a work in progress and our goal is to make it user friendly and helpful for all chemical researchers out there.

April 10, 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

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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

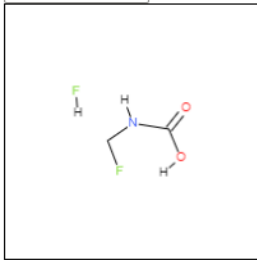
Map Search

atoms ▾

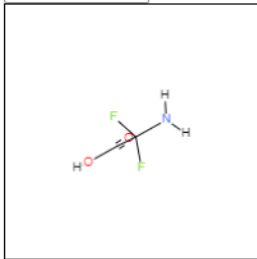
Sort: ▾ Order: ▾

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

User's Manual

So now you sit in front of your computer with the browser open and the SCAN 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 SCAN in your research and work, how to load data-maps, how you can study them in various way. How you can open and analyze the node graph and find out more details about each node and edge of the chemical reaction data. Whether you will discover something new is more up to you though and not the scope of this manual. We are software developers and not chemist, but by providing you with this tool we hope that your trained eyes and extensive knowledge will help you perhaps see something new that you have not seen before and take it from there. Let's teach you how to use this web tool to the fullest.

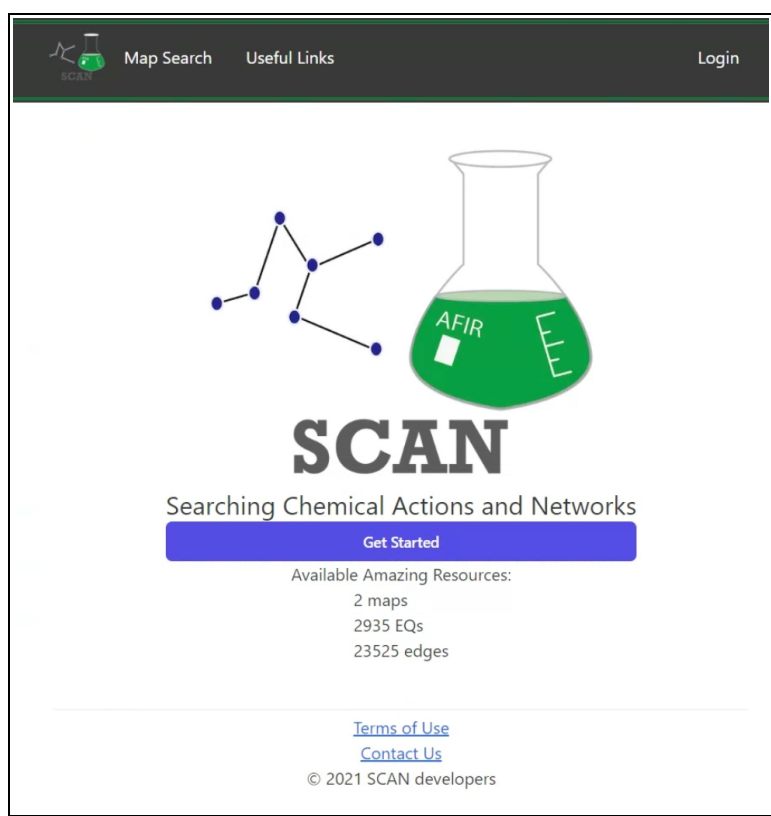


Figure 1: This is the first view that a SCAN visitor is met by

SCAN Front Page

The first thing a SCAN Web application visitor sees is the SCAN Front Page as can be seen in Figure 1. At the top is the top menu with its available options which will be present during the whole SCAN visit for simple and quick navigation. Below that is the SCAN Logo and full application name. Below that is a quick access button to the reaction map search area just above some information about the currently available amount of data stored in the SCAN Database. At the bottom of the page one can find a link to the 'Terms of Use' page and a 'Contact Us'-link to the SCAN development team's mail address for support and other queries.

SCAN Top Menu

SCAN's top menu (as seen in Figure 2) is small and effective with basically only 4 choices, and in practicality one could say there is only one real choice.

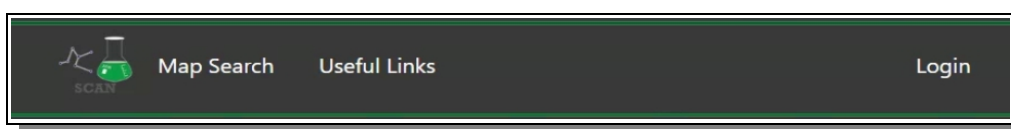


Figure 2: The Top Main Menu for the SCAN Web Application

The small SCAN logo to the left is a clickable link for returning to the original Start Front Page, Home so to speak. The 'Map Search' takes the user to the page where one can search for any of the available reaction maps. 'Useful Links' is taking the user to a list of useful links and documents that might be of use. The last menu item, far to the right is the 'Login' (or if already logged in, the 'Logout') option.

It is required for the user to be logged in and have a proper SCAN account in order to access any of the data and tools of the web application.

Scan Front Page Footer

At the bottom of the front page of SCAN, there is a small footer (as seen in Figure 3) with some useful information and access point.

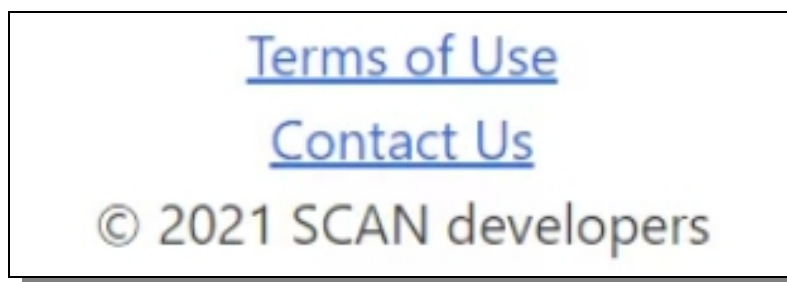
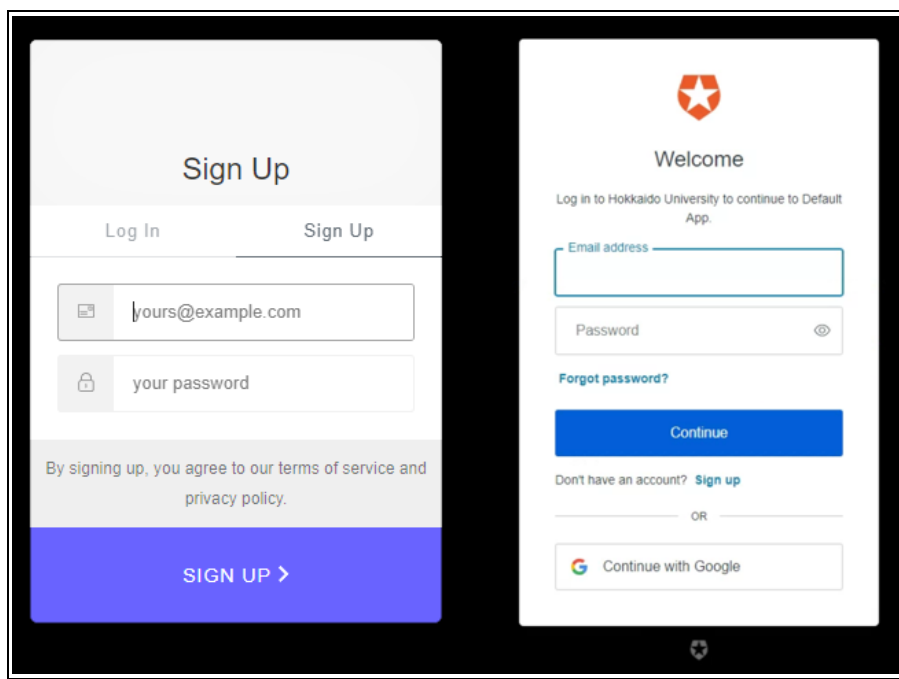


Figure 3: The footer links are only available at the first front page.

The 'Terms of Use' link will take the user to a page displaying all legal issues regarding the use of the SCAN web application, while the 'Contact Us' link will open the user's associated mail-program and let the user send a mail to the SCAN development team about whatever is on their mind.

Login and User Accounts

When a user visits the SCAN web application for the first time, they need to create a SCAN account in order to be let in any further. To do that one just clicks the 'Login' menu item at the top of the application which will then replace the current view with a Login/Sign Up view (as illustrated in Figure 4 below).



1. Figure 4: To the left is the Sign Up form, and for returning users the Login form to the right will be used.

Creating an account is fast and easy, and the user will be immediately signed in after the creation has been registered without any further hassle. It is important to use a valid mail address though, especially if one forgets the password and requests to be sent a mail to change it. Login for returning users is equally easy as can see in the figure above, with an option to bind the account to ones Google account if so wanted. As soon as the login has been approved by the authentication system the user are promptly returned to the front page of the SCAN Web Application, with the only difference that no the top right corner of the main menu says 'Logout' as a n option instead of previously 'Login' as can be seen below in Figure 5.

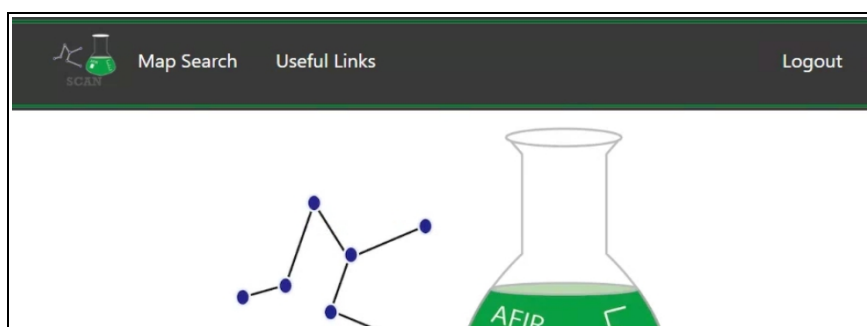


Figure 5: If the user was previously and recently logged in, they will be automatically logged in again.

Map Search Page

It is on the Map Search page where the real fun begins and where one usually goes with speed after loading the SCAN web application. The Map Search page basically contains of a small and simple search form as can be seen below in Figure 6.

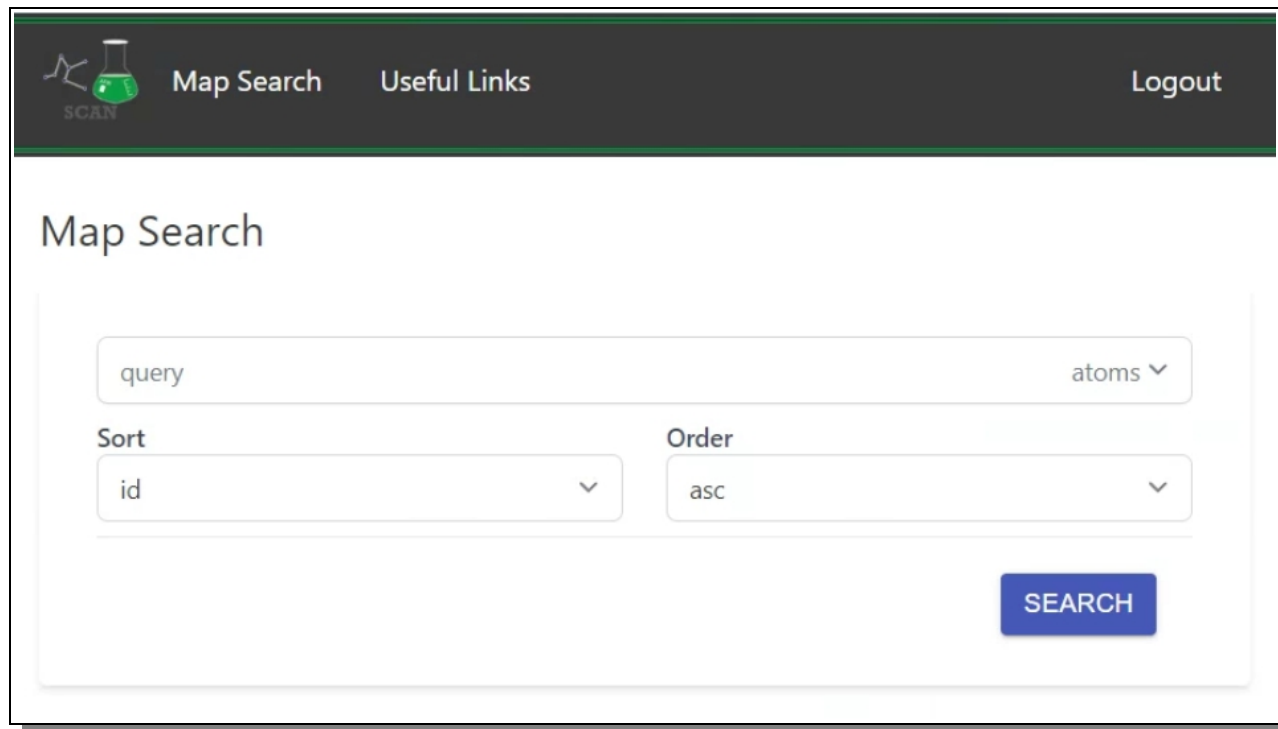


Figure 6: The Scan Map Search is the entry point for going further in to explore what SCAN has to offer.

In the query field the user can type any atom they are interested in and search to see if there are any maps that contains that atom. After a short while after filling in the query field and clicked 'Search', the result containing a list of reaction maps will appear below, as can be seen in Figure 7.

Each item in the list is a reaction map for a specific molecule, where the molecule's chemical description at the top, to the right, is the name of the reaction map and also the clickable link to get to that specific map. Below are some other useful attributes that describes the map, such as internal database ID (good for exact reference), a list of containing atoms, the lowest energy value for one version of the molecule as well as the highest energy value for another version. Also showing is the number of EQs, nodes in the map, meaning versions of the base molecule, and the number of TSs, edges or links, that is paths a molecule can take to transform into another version. Information when the map was created and updated is also available at the end. To the left of the item block is an interactive 3D model of the molecule, that can be rotated and viewed by using the mouse inside the dedicated square.

If the result list is long, the user can sort and order the list based on any of the multiple available attributes the map contains, in order to easier find the map they are looking for, as can be seen in Figure 8.

The 'Switch View' button as can be seen at the top of each 3D molecule in e.g. Figure 7 can be clicked and it will then change how the molecule is being displayed. The second view is still 3D, but have a bit more colorful and 2D feel to it as can be noticed in Figure 9.

Map Search

C atoms ▾

Sort: id ▾ Order: asc ▾

SEARCH

Results: 2 map found.

switch view

NC(=O)N.O.O
Id: 01FKZ1SHNKGVCSTB9727XAKERS
Atoms: O,C,N,H,H,N,H,H,O,H,H,O,H,H
Lowest_energy: -377.61648301912
highest_energy: -377.2944551885
EQs: 1159, **TSs:** 12156
 Created: November 8, 2021
 Updated: November 8, 2021

switch view

NC(=O)N.O.O
Id: 01FKZV7J81R92AG1YRBGFQWRS
Atoms: O,C,N,H,H,N,H,H,O,H,H,O,H,H
Lowest_energy: -377.773878213754
highest_energy: -377.254546715411
EQs: 1776, **TSs:** 11369
 Created: November 8, 2021
 Updated: November 8, 2021

Showing 1 to 2 of 2 results

Figure 7: The Search result showing the reaction maps that contains the chosen atom.

Sort: id ▾ Order: asc ▾

id
 atom_name
 inityz
 fname_top_abs
 fname_top_rel
 natoms
 lowest_energy
 highest_energy
 neq
 nts
 npt
 jobtime
 universal_gamma
 infile
 scpathpara
 jobtype
 pathtype
 nobondrearrange
 siml_tempearture_kelvin
 siml_pressure_atm

asc
 desc

SEARCH

Figure 8: The reaction map search result can be both sorted and ordered based attributes.

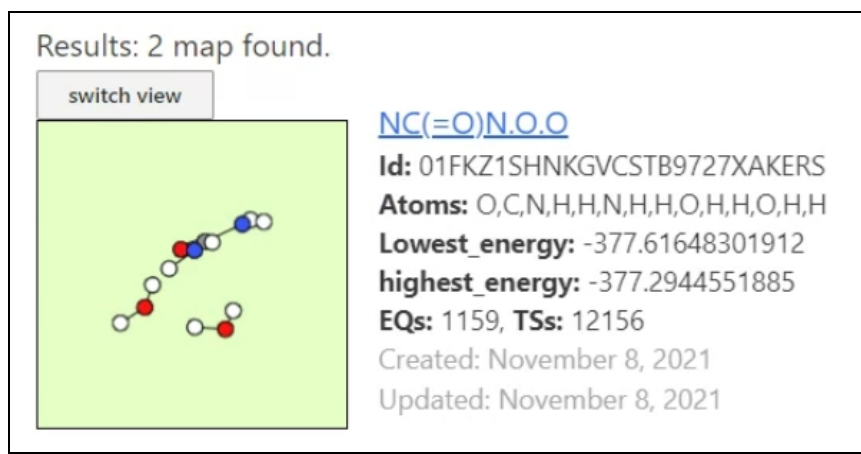


Figure 9: There are two types of views to use when looking at the 3D molecule.

When the user have decided which map they wish to look closer at, they click the blue molecule name link, and will then be transported to the Reaction Map Detailed View Page.

Map Detailed View

After clicking on a specific map one is sent to a page showing all the available attributes that a map contains. An example of such a map info page can be seen in Figure 10.

Below some of the more important ones of those attributes are described in more detail.

SOME REACTION MAP ATTRIBUTES

atom_name

These are all the names of the containing atoms.

natoms

This is the number of atoms present in the molecule.

lowest_energy

This is the lowest energy value present in the reaction map

highest_energy

This is the highest energy value present in the reaction map

neq

This is the number of nodes present in the reaction map, the number of possible variants of the molecule. The value is clickable and will take the user to a new page listing all nodes individually.

npt

This is the number of edges (links) present in the reaction map, the number of possible paths to get from one molecule variant to another. The value is clickable and will take the user to a new page listing all edges individually.

siml_temperature_kelvin

Which degrees of Kelvin were used for the different versions of the map

[Go to GraphViewer](#)

NC(=O)N.O.O
id: 01FKZ1SHNKGVCS1897Z7XAKERS

| | |
|-------------------------|---|
| atom_name | ['O','C','N','H','H','N','H','H','O','H','O','H','H'] |
| natoms | 14 |
| lowest_energy | -377.61648301912 |
| highest_energy | -377.2944551885 |
| neq | 1159 |
| nts | 0 |
| npt | 12156 |
| jobtime | 2021-09-13T09:50:35 |
| universal_gamma | 100 |
| infile | none |
| scpathpara | none |
| jobtype | sc-afir |
| pathtype | luppath |
| nobondrearrange | 0 |
| siml_temperature_kelvin | [200,300,400] |
| siml_pressure_atm | 1 |
| level | wb97xd/sv |
| spinmulti | 1 |
| totalcharge | 0 |
| jobstatus | finished |
| ngradient | 4049988 |
| nhessian | 118978 |
| elapsedtime_sec | 112936 |
| registrant | |
| creator | |
| created_at | 2021-11-08T14:54:48 |
| updated_at | 2021-11-08T14:54:48 |

[Go to GraphViewer](#) [Download Graph as CSV](#)

Figure 10: The full list of attributes that is contained within each reaction map.

At the bottom of the attribute list there is a button that allows you to download the complete reaction map as a CSV file, if you wish to study it in some other way and/or with some other tools.

At both the top and at the bottom there is also a clickable link that says 'Go to Graph Viewer', which if

clicked will do just that for even more exciting ways to study the reaction map.

Map Nodes View

The Nodes List view Page, basically reached from the Map Details Page, contains of a list of every molecule contained inside the reaction map. Each molecule is shown with a few key attributes and a 3D visualization view-port that shows the specific molecule. An example of such list can be seen in Figure 11.

The screenshot shows a web interface titled "EQ List in: NC(=O)N.O.O" with a sub-header "# 01EKZ15HNKGVCSTB97ZXAERS". It displays "Showing 1 to 50 of 1159 results". The interface includes a "Sort" dropdown set to "id" and a "Number of items" dropdown set to "50". The list contains 15 entries, each with a "switch view" button, a 3D molecular model, and the following text:

- EQ-6**: #E:01FKZ15HNK32818R0933930VV, Category: eq, Energy: -377.590700315416, Canonical SMILES: NC(=O)N.O.O
- EQ-5**: #E:01FKZ15HNK309V78EER305GMS3, Category: eq, Energy: -377.599646321518, Canonical SMILES: NC(=O)N.O.O
- EQ-0**: #E:01FKZ15HNK309P92008515, Category: eq, Energy: -377.599102935747, Canonical SMILES: NC(=O)N.O.O
- EQ-7**: #E:01FKZ15HNK309B46327AD49D74, Category: eq, Energy: -377.59594438347, Canonical SMILES: NC(=O)N.O.O
- EQ-3**: #E:01FKZ15HNK3097022F12V95WS1, Category: eq, Energy: -377.607802473233, Canonical SMILES: NC(=O)N.O.O
- EQ-1**: #E:01FKZ15HNK309M9DF3Y2Z09P, Category: eq, Energy: -377.598851712813, Canonical SMILES: NC(=O)N.O.O
- EQ-4**: #E:01FKZ15HNK309N6V66W4H45, Category: eq, Energy: -377.590384348416, Canonical SMILES: NC(=O)N.O.O
- EQ-2**: #E:01FKZ15HNK309G200CV5FK80D, Category: eq, Energy: -377.59183827251, Canonical SMILES: NC(=O)N.O.O
- EQ-11**: #E:01FKZ15HNK309T7W5CDH15BM7N1, Category: eq, Energy: -377.591369669236, Canonical SMILES: NC(=O)N.O.O
- EQ-8**: #E:01FKZ15HNK309A40779N4R9V29W0V, Category: eq, Energy: -377.60033974620, Canonical SMILES: NC(=O)N.O.O
- EQ-17**: #E:01FKZ15HNK309M9Y69898NCR, Category: eq, Energy: -377.604516004937, Canonical SMILES: NC(=O)N.O.O
- EQ-13**: #E:01FKZ15HNK309H1142N80V39KCF, Category: eq, Energy: -377.634637642043, Canonical SMILES: NC(=O)N.O.O
- EQ-18**: #E:01FKZ15HNK309M75M6W0XMM84FC, Category: eq, Energy: -377.600800776240, Canonical SMILES: NC(=O)N.O.O

Figure 11: A list of all individual nodes in the reaction map

At the top of the screen is shown the name and id of the reaction map, and just above the node/molecule list display, is an option to sort the list by energy instead of id number as can be seen in Figure 12, as well as to choose how many to display per page.

The screenshot shows the same web interface as Figure 11, but the "Sort" dropdown is set to "energy". The list contains 15 entries, each with a "switch view" button, a 3D molecular model, and the following text:

- EQ-808**: #E:01FKZ15HNK309I7V9CA5G39K147, Category: eq, Energy: -377.2944551885, Canonical SMILES: [N]C(=O)N.[H]O.O.O
- EQ-332**: #E:01FKZ15HNK309E3Q9D8K2068MVG, Category: eq, Energy: -377.320684007811, Canonical SMILES: [C]3[N]O.N.O.O
- EQ-183**: #E:01FKZ15HNK309H02P9H0D0V0CB31, Category: eq, Energy: -377.321367888006, Canonical SMILES: [C]3[N]O.N.O.O
- EQ-328**: #E:01FKZ15HNK309Y13Q9MA684K11, Category: eq, Energy: -377.32262071343, Canonical SMILES: [C]3[N]O.N.O.O
- EQ-742**: #E:01FKZ15HNK309V92V6W7G0KMS25, Category: eq, Energy: -377.322764790396, Canonical SMILES: [H]C(=O)N.[H]O.O.O
- EQ-256**: #E:01FKZ15HNK309T7F684T255790A, Category: eq, Energy: -377.32416506958, Canonical SMILES: [C]3[N]O.N.O.N
- EQ-214**: #E:01FKZ15HNK309S8B9Y7V29148R2, Category: eq, Energy: -377.32500730472, Canonical SMILES: [C]3[N]O.N.O.N
- EQ-419**: #E:01FKZ15HNK309Y7CE2B34YXG8D, Category: eq, Energy: -377.32018002161, Canonical SMILES: [C]3[N]O.N.O.O
- EQ-196**: #E:01FKZ15HNK309H24YTA1WZCP0W2, Category: eq, Energy: -377.34054104795, Canonical SMILES: [C]1NCO1.O.O.N
- EQ-1128**: #E:01FKZ15HNK309V9Y0C2B2CFQR, Category: eq, Energy: -377.355193861311, Canonical SMILES: O=C.[N]([H])[O].O.O
- EQ-814**: #E:01FKZ15HNK309I35C972D8X0Z02, Category: eq, Energy: -377.356472324489, Canonical SMILES: NC(=O)N.O.O
- EQ-726**: #E:01FKZ15HNK309P00E4723748V70Z5, Category: eq, Energy: -377.358618089544, Canonical SMILES: NC(=O)N.O.O
- EQ-722**: #E:01FKZ15HNK309Y707E2M9W0ACMX3, Category: eq, Energy: -377.361009964152, Canonical SMILES: NC(=O)N.O.O
- EQ-796**: #E:01FKZ15HNK309W0AD4H0Y4R2Z05V, Category: eq, Energy: -377.362870175635, Canonical SMILES: NC(=O)N.O.O
- EQ-303**: #E:01FKZ15HNK309F32W08C0KCAJZ8, Category: eq, Energy: -377.363833573158, Canonical SMILES: NC(=O)N.O.O

Figure 12: The nodes list sorted by energy values instead

If any of the displayed molecule 'nodes' are clicked on its id link, the user is transported to view that specific molecule's detailed data.

Node Detailed View

After clicking on a specific molecule reaction map node, one is sent to a page showing all the available attributes that the chosen molecule map node contains. An example of such a node info page can be seen in Figure 13.

There are 17 attributes shown on the site page, but all are not equally as important, so below is shown

SCAN User Manual

some further detailed information only for those that are of more importance.

| | |
|--|--|
| EQ: 808 id: 01FKZ1SHQ1TV9CA5G58KJET47 | |
| Structure | <div style="text-align: center;">switch view Download XYZ file</div> |
| nid | 808 |
| category | eq |
| symmetry | C1 |
| xyz | <pre>[[-3.477839995315067, 1.9964013042386108, -1.853569992554612], [-3.7692219988561906, 1.9324879701772656, 1.0095283463688742], [-1.495665775812671, 2.2311234448308643, 1.9041466328874619], [0.2556813040410965, 2.22690215013571, 0.8438129869789622], [1.1186812869632647, -1.732099229039229, 4.605906234062228], [-2.606439044744344, -0.1490775557661966, -3.1104783459936693], [-0.9369453026428203, -2.0264717883912655, -1.6182259874592606], [0.9235809082223034, -1.9177671749962175, 3.194089228913543], [2.6241515921671836, 1.426990073579297, -0.4876300613690971], [2.342393318746022, -0.47508643539775464, -0.668799427939881], [3.5153231373898315, 2.198384036956207, -1.8923280914387914], [0.7036003706841145, -2.78348526044248, -0.9078967651496563], [-1.3114648660415105, 2.2240078688568112, 3.8184660518729143], [0.6496307249596062, -4.540543773179106, -0.392507202032036]]</pre> |
| energy | [-377.2944551885, -377.166657225789.0] |
| gradient | |
| s2_value | 0 |
| dipole | |
| comment | EQ808 |
| hess_eigenvalue_au | [0.000193494, 0.000386247, 0.000534637, 0.000750126, 0.000860893, 0.001574393, 0.002556303, ...] |
| trafficvolume | [0.0.0] |
| population | [null,null,null] |
| reactionyield | [0.0.0] |
| created_at | 2021-11-08T14:54:56 |
| updated_at | 2021-11-08T14:54:56 |
| map_id | 01FKZ1SHKGVCSB9727XAKERS |

Figure 13: The detailed view of a specific molecule, reaction map node, with all its data attributes.

SOME NODE ATTRIBUTES

Structure

This is a molecule 3D visualization for the map node, with an option to switch display style as well as an option to download the xyz data for the molecule to be used or shared externally.

Nid

Node Id, for easy identification.

category

eq is the category identification for nodes

xyz

the xyz format that describes the molecule in 3D space.

energy

the energy value for this molecule

gradient

the molecule gradient concentration

dipole

the molecule dipole moment value if present

hess_eigenvalue_au

The Hessian eigenvalue for this node

reactionyield

the yield amount this specific molecule is produced in a reaction.

Map Edges View

The Edge List view Page, basically reached from the Map Details Page, contains of a list of every link/path from one molecule to another, contained inside the reaction map. Each link is shown with a few key attributes and a 3D visualization view-port that shows the specific molecules involved. An example of such list can be seen in Figure 14.

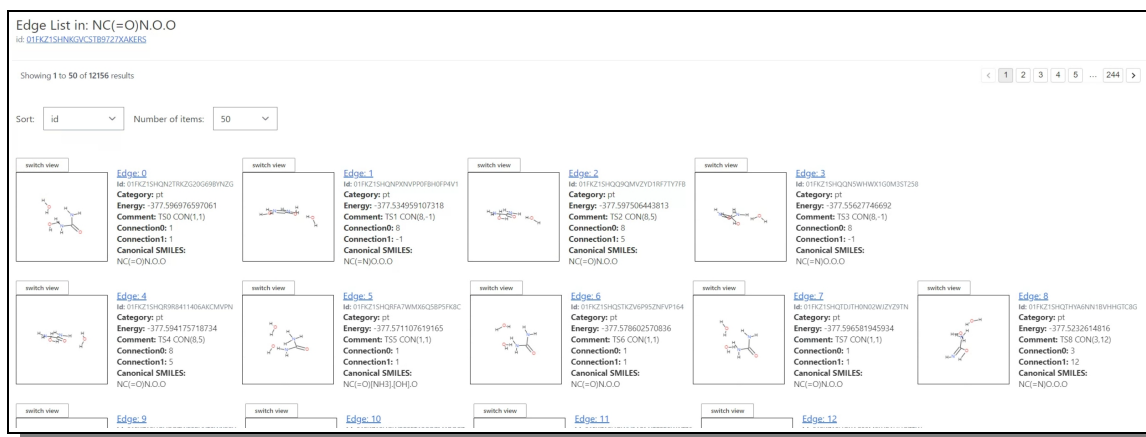


Figure 14: The list of edges this reaction map contains.

At the top of the screen is shown the name and id of the reaction map, and just above the edge/link/path list display, is an option to sort the list by energy or connection instead of id number as.

If any of the displayed 'edges' are clicked on its id link, the user is transported to view that specific edge path's detailed data.

Edge Detailed View

After clicking on a specific molecule reaction map edge/link, one is sent to a page showing all the available attributes that the chosen molecule map edge contains. An example of such a edge info page can be seen in Figure 15.

There are 16 attributes shown on the site page, but all are not equally as important, so below is shown some further detailed information only for those that are of more importance.

Edge: 6463
id: 01FKZ1SS0KCIH3G4TZ4ADCKZW0

Structure

switch view

Download XYZ file

| | |
|--------------------|--|
| edge_id | 6463 |
| category | pt |
| symmetry | C1 |
| xyz | [[[-0.4818328044730434,-2.1091064711079444,-2.729034671067274], [-1.8729221459726815,0.19713477614189723,2.158595829523276], [-0.8759015523964826,2.3766935496805535,2.554137233441417], [-1.1279643068498586,2.23944277510124,-0.6752121487785278], [0.995229582782006,2.231145320021118,3.0731665176501193], [-0.7050857817868885,-2.1402453485920745,2.275986746359536], [-3.8088953264523284,0.062447695384576146,1.4450352872086534], [-0.972903780315393,-3.0658340741156844,0.5628211614724956], [1.9797263174819522,-1.8626072027257543,2.58771606009086], [2.4014835874189293,-2.847402124113238,4.09221820459632], [-0.3721078090471724,-2.3767944745920095,-3.0201911346627073], [-1.106745045866475,2.727547058167272,-2.4976784782503], [-1.872786847166591,3.961804820433616,-3.6160365711886455], [-0.6609676141008851,-0.26348789450318943,-2.8775346949619145]]] |
| energy | [-369.953169333922,-369.826102663697,0] |
| gradient | |
| s2_value | 0 |
| dipole | |
| comment | TS6463 CON(560,456) |
| hess_eigenvalue_au | [-87.097039875,-85.968539902,0.000001003,0.00022038,0.000603462,0.0006552,0.002401591 |
| connection0 | 560 |
| connection1 | 456 |
| created_at | 2021-11-08T14:54:55 |
| updated_at | 2021-11-08T14:54:55 |
| map_id | 01FKZ1SHINKGVCSTB9727XAKERS |

Figure 15: The detailed view of a specific path, reaction map edge, with all its data attributes.

SOME EDGE ATTRIBUTES

Structure

This is a molecule 3D visualization for the map edge, with an option to switch display style as well as an option to download the xyz data for the molecule to be used or shared externally.

edge_id

Edge Id, for easy identification.

category

pt is the category identification for edges

xyz

the xyz format that describes the molecule in 3D space.

energy

the energy value for this reaction path

gradient

the gradient concentration

dipole

the dipole moment value if present

hess_eigenvalue_au

The Hessian eigenvalue for this reaction path

connection

connection0 and conection1 are the ids of the two nodes that this edge connects.

Map Graph View

When one clicks on 'Go to GraphViewer' the view switches and a new interface is loaded below the application main menu, which contains of a simple upper sub menu, some instructions and buttons and a large drawing area where the reaction map data will be displayed as a network graph with nodes and links, representing all molecules and their transforming paths .

The default network is drawn immediately and it is weighted by the nodes energy values, where the higher energy value (closer to 0) is of a more red (warm) color and lower (more negative) is of a more blue (cold) color. An example of this view can be seen in Figure 16.

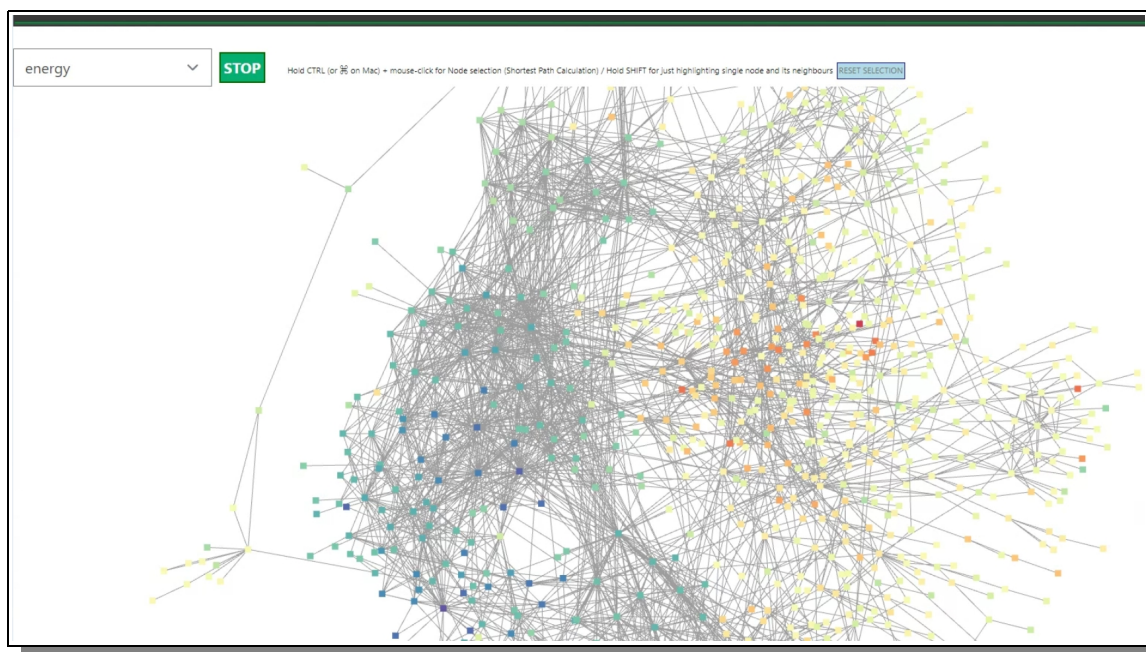


Figure 16: The Reaction map displayed as a node graph with each molecule node and its connections edges.

What one will quickly notice is that all the nodes and the whole map is shaking, quite violently. This is because the network graph is trying to adjust each node's position according to its base setting for gravity and such between nodes. If one wish to wait for it to finish by itself, it might take quite a while, so therefore there is a green button that says 'STOP' at the top and which will hold the current position for each node. In this state the user can manually move the nodes individually with drag and drop. The green button then change to 'RESUME', which naturally allows the user to resume the auto location correction feature to begin again if wanted. The Figure 17 shows this state.

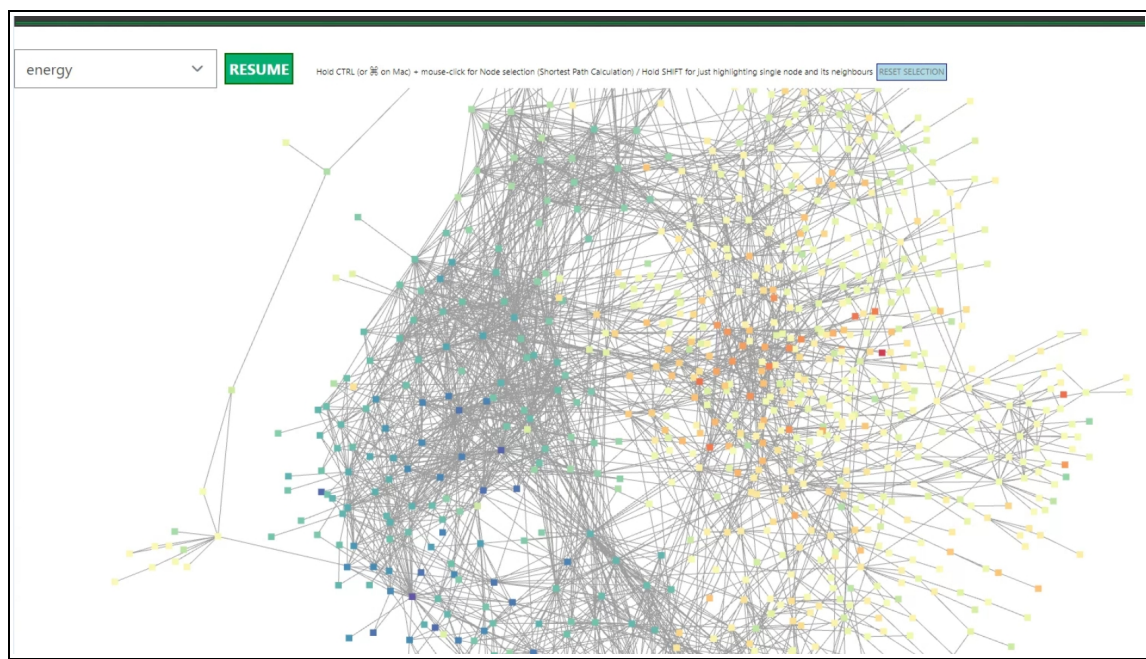


Figure 17: After the auto adjusting of nodes have stopped, each can be manually moved.

Basic Interactions

The base interaction a user can do with the network graph as a whole is to pan it by dragging the mouse in the white area and zoom with the mouse wheel.

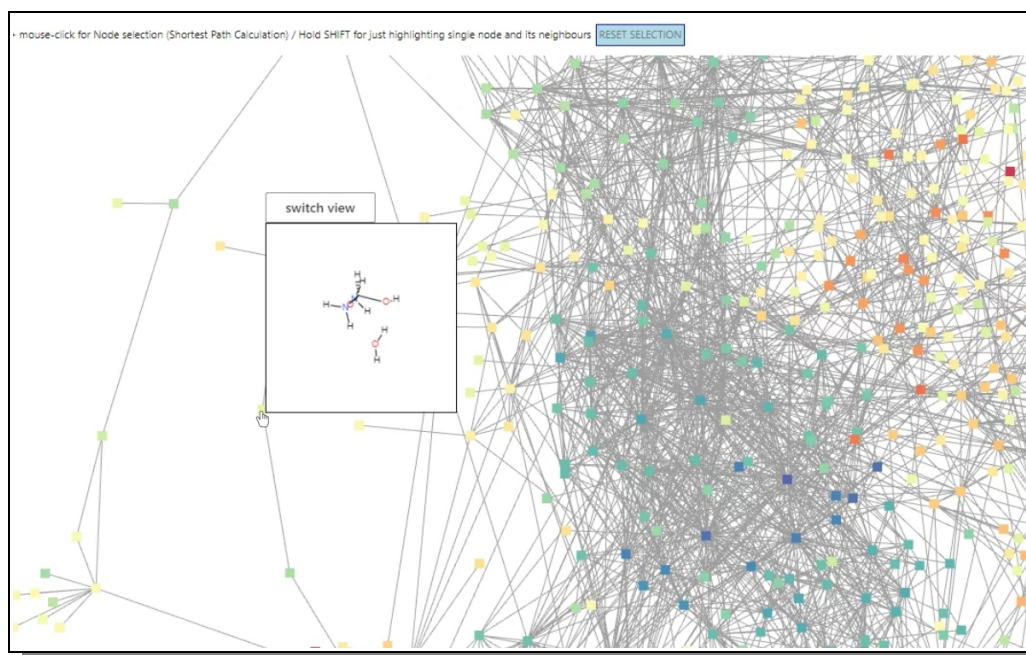


Figure 18: When hover the mouse above a node it shows the molecule 3D view which the user can interact with.

In Figure 18 we can see how a popup window shows up as we hover above a specific node and show us an interactive 3D view-port of that node's molecule. Using the mouse one can rotate the molecule freely and with the 'Switch View' button the style of the molecule drawing changes.

If one double click on a node a new tab will open showing the selected node's detailed info page as mentioned before and seen in Figure 13.

The color and size of a node is informative and relevant, but what it exactly means depend on which mode the network graph is currently shown in, which will be further explained further on.

Advanced Interactions

How these interactions are done are also explained, in simple words, in the instructions above the network graph for better help and support.

Node Selection

If one clicks on a node while holding the SHIFT-key, the node will be selected (grow in size and turn yellow). All neighbouring nodes connected to the selected node will also be semi selected (grow in size and turn pink) for the user to easily track relationships. This can be seen in Figure 19.

Shortest Path Selection

If one instead clicks a node while holding the CTRL-key (or the mac-key on an Apple computer) one initiate the process of calculating the shortest path between two nodes. The one clicked on will turn yellow and the system is now waiting for the user to CTRL-click yet another node. The user can then pick any other node and click on it while holding the CTRL-key.

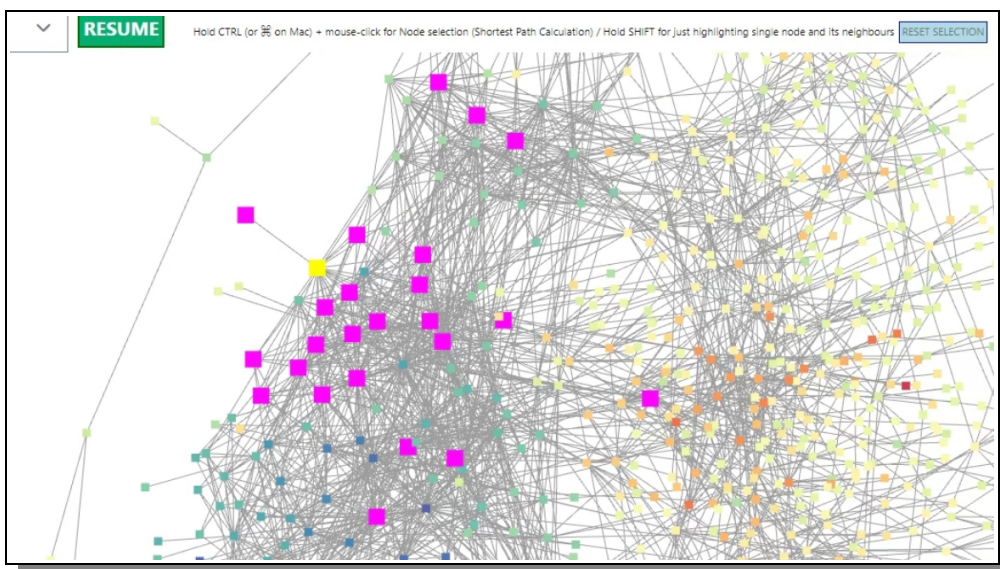


Figure 19: A node and its neighbours selected.

As soon as that is done the system will then calculate the shortest path from the first node to the final node. Mark them all in pink colors and add a number to each node starting with 1 on the first clicked node and then so forth. The user can now see the shortest path between two nodes, which other nodes are involved and how many of them. An example of this can be seen in Figure 20

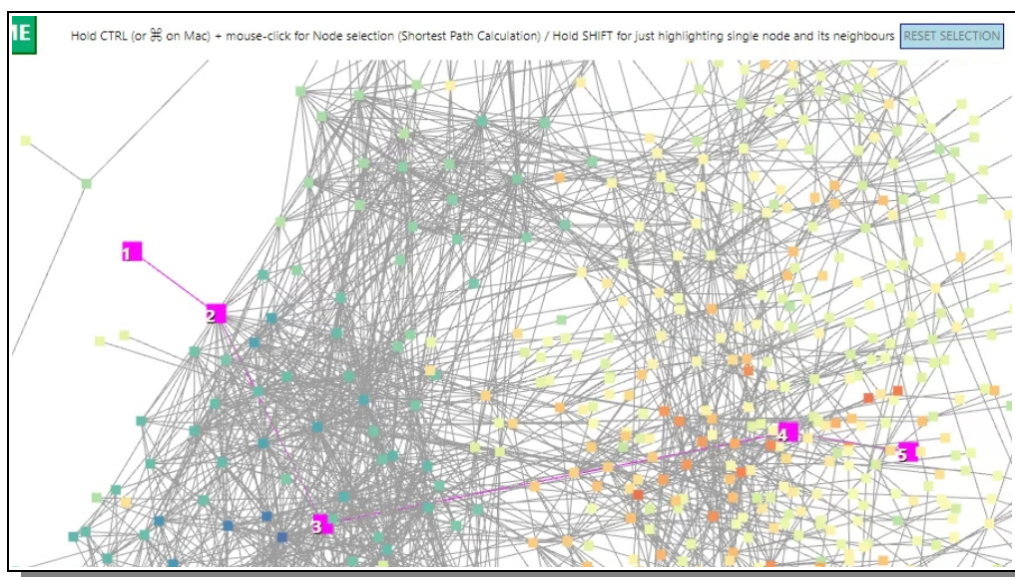


Figure 20: The shortest path between two nodes.

Deselect

To deselect all current selected nodes the user just needs to click the light blue button above the network graph named 'RESET SELECTION', and then the graph goes back to default state and all ready to have other nodes selected instead.

Graph Drawing Modes

To the left above the network graph is a drop down box that allows the user to change how the network should be weighted and structured. The top-most default setting is 'Energy' which uses the reaction

map's energy values is weights for the network graph. As have already been shown in Figure 16 and Figure 17.

The other modes can be seen in Figure 21, and are further explained below. In Figure 22 one can see one other example of such a different mode of calculating and drawing the network graph.

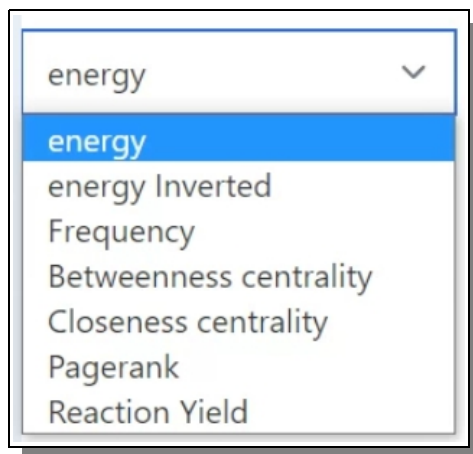


Figure 21: The different Graph drawing modes available.

AVAILABLE GRAPH DRAWING MODES

Energy

the energy value for each molecule node is used as weights and the colors range from lower to middle to higher as from blue to yellow to red.

Energy Inverted

The same weights are used but in this case the colors are inverted so the lower values are more red and the highrte values are more blue. This is for a more convenient identification of the molecules that are of interest.

Frequency

This mode draws the graph based on how often a molecule appears.

Betweenness Centrality

This mode is a measure of a node's importance. It is based on the idea that a node is important if it lies on many shortest paths between other nodes in the network. The betweenness centrality of a node is defined as the number of shortest paths between all pairs of nodes in the network that pass through that node.

Closeness Centrality

This mode is another measure of a node's importance. It is based on

the idea that a node is important if it can reach other nodes in the network quickly, either directly or indirectly.

Pagerank

This mode assigns a score to each node in the network based on the structure of the network and the links between nodes. The basic idea is that a node is more important if it is linked to by other important nodes in the network.

Reaction Yield

This mode uses the yield values as weights for the network graph. This mode also have some additional settings as explained below.

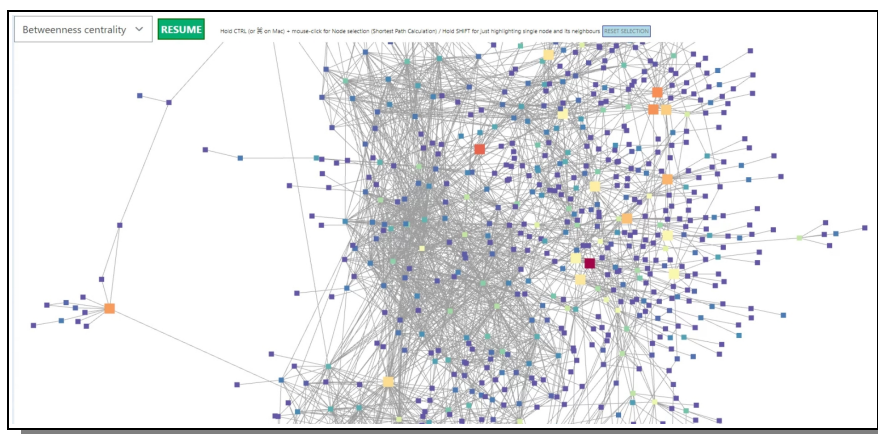


Figure 22: Using a different graph drawing mode, in this example the Betweenness Centrality calculation.

How each mode is used, read and interpreted is very much up to the user/researcher studying the network graph, and it is all up to them how they take what they see and find further.

The only mode that slightly differ from the other modes is the last 'Reaction Yield' mode, since it contains a few more settings to play around with as explained below and can be seen in Figure 23.

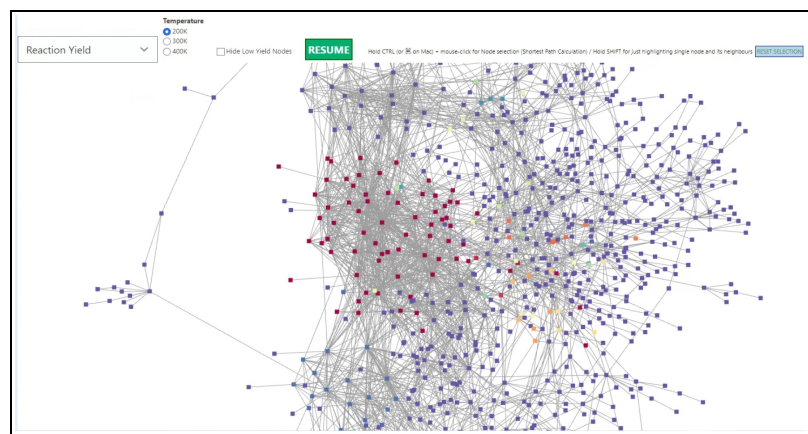


Figure 23: The default Reaction Yield Network graph.

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The first setting (radio buttons) is based on the temperature applied to the reaction, either 200, 300 or 400 K (Kelvin) and draws the high yield nodes with a more warm and red color and the low or no yield nodes with a cooler and blue color. Changing the temperature change the yield amount of the graph nodes, as can be seen and compared in Figure 24.

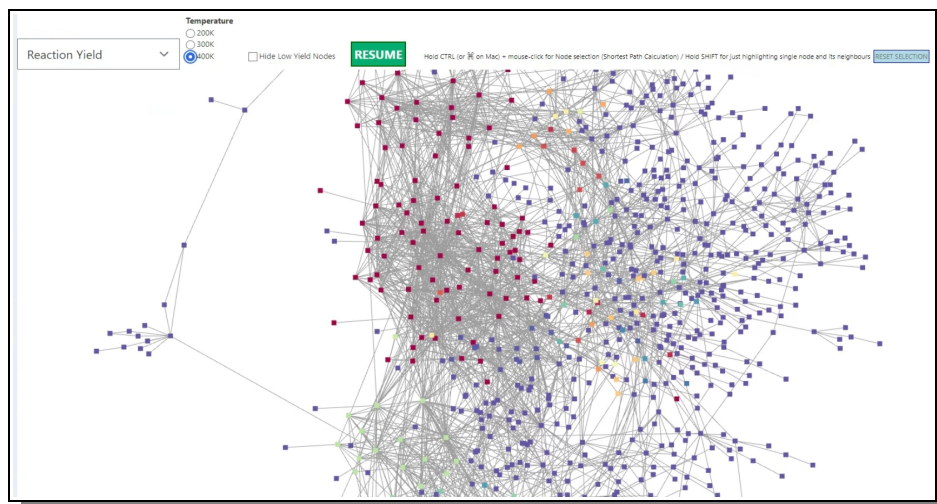


Figure 24: The yield values in a 400K reaction

The second setting (check box) allows the user to hide all low yield nodes and its edges for a less cluttered view and better focus on nodes of importance. An example of this can be seen in Figure 25.

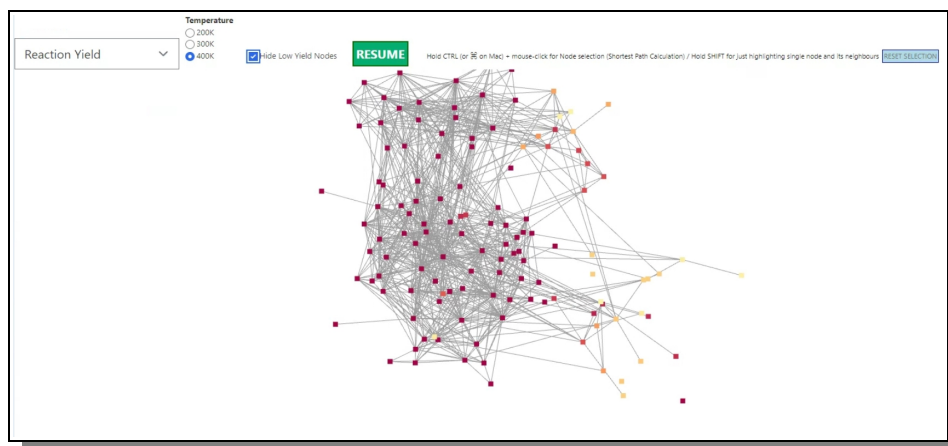


Figure 25: Only show high yield nodes and hide the rest.

Summary

We wish that this manual have told you anything and everything you need to know about SCAN Web application and how to use it. Feel free to return here whenever your memory fails you on what to do and when.

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



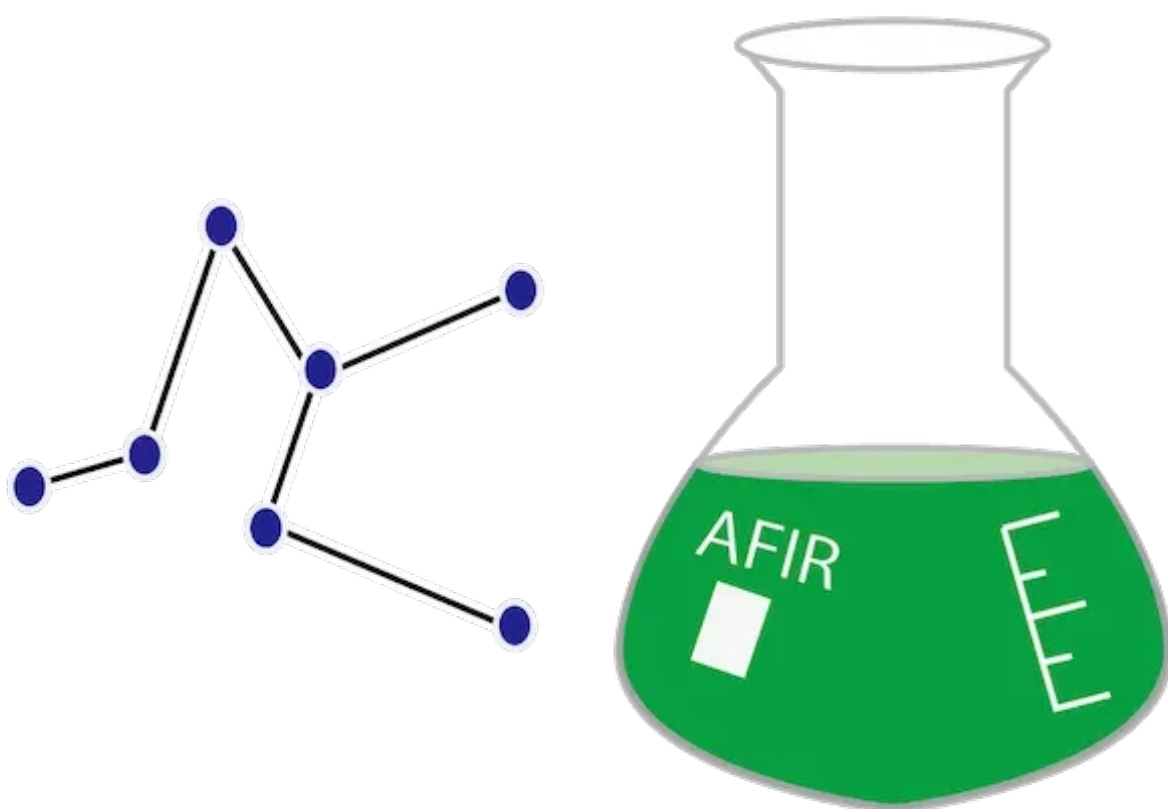
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Thanks for your support



SCAN