

Main page

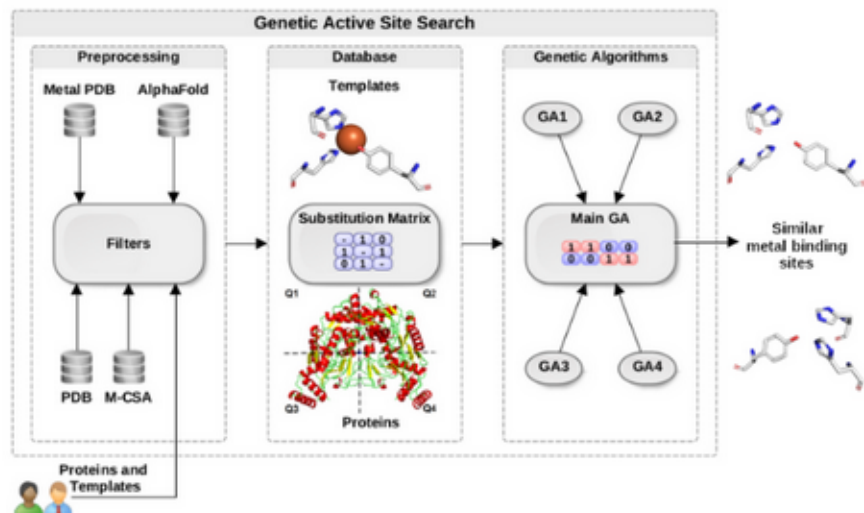
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1 **2**

GASS-Metal

GASS-Metal is a method based on a genetic algorithm to search for similar metal-binding sites in proteins. In addition to finding similar metal-binding sites, the method can find inter-domain sites and perform not exact matches using a substitution matrix (conservative mutations).

In this new version, **GASS-Metal** uses parallel genetic algorithms to create an initial population (seeds), improve accuracy and decrease processing time.



About GASS-Metal

GASS-Metal is a user-friendly web server based on parallel genetic algorithms to predict metal-binding sites in protein structures, based on similarity of known sites. It has two available resources:

- **Metal-binding Site Search (1):** Given a protein of interest, try to match a metal site based on M-CSA and MetalPDB.
- **One-to-one Site Search (2):** The user can give the protein target and your template.

Metal-binding Site Search

Metal-binding Site Search

GASS-Metal

Step 1

Please provide a target protein structure (PDB format):

Upload your own PDB file:

Choose PDB file

1 Or

Provide a 4-letter PDB code or UniProt code (AlphaFold):

Step 2

Please select the metal ion templates:

Choose the basic metal ion, a type of metal-binding site and template size.

Select one of the following metal ions:

2

Select a type of metal-binding site:

3

Select template size (number of residues):

4

Step 3

Please select the reference atom:

5

Please choose the conservative mutations:

6

7

8

Disclaimer: No PDB files will be retained on the system after being uploaded by the user. ✕

How to run Metal-binding Site Search

To perform a site search based on **M-CSA** and **MetalPDB**:

- **Step 1:** The user must provide a 4-letter PDB code or UniProt code (AlphaFold), or provide a PDB file (**1**), which will serve as a target for searching metal-binding sites. It is in this protein that GASS-Metal will search for similar sites using its templates.
- **Step 2:** Where the templates on which the search for GASS-Metal will be based are filtered. Users must first choose the metallic ion of the site (**2**), the type of this site (if it is simple, containing only one ion, or compound, having two or more metal ions) (**3**) and the number of residues that make up the templates (**4**). The **All** option enables GASS-Metal to perform an exploratory search considering all templates for that metal ion.
- **Step 3:** The user can choose between the alpha carbon or the last heavy atom (LHA) as the reference atom in the templates (**5**). The user also can choose one of three options about conservative mutations (**6**): use mutations provided by GASS-Metal, use user-defined mutations or use no mutations at all.

Finally, click on the button **Run GASS (7)** to perform the search.

The button **Run Example (8)** will perform a metal-binding site search based on a pre-defined example.

Processing Page

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Processing results for job csa_1633125413.45

Your request is being processed by the GASS-Metal webserver, it may take some minutes depending on the total number of templates being used and the numbers of requests to server.

You may reload this page check if the results are already available, or save the link to check results later.

The results will be available through this link for 15 days.

1

https://gassmetal.unifei.edu.br/prediction/csa_1633125413.45/mbs

Click to copy to clipboard



Best viewed using [Chrome](#) on 1280x1024 resolution and above

Processing Page

A request made to the GASS-Metal web server may take a few minutes depending on the total number of templates being used and server load.

Users may reload the results page to check if the results are already available or save the link to check results later **(1)**.

The results will be available through the link for 15 days.

Results page

Visualization controls

Show template properties **1**

Predicted metal-binding sites

Job ID: csa_1633125413.45mbs **2**

10 records per page Search:

| Index | Fitness | Found metal-binding site on query PDB | Template PDB ID | Matched template on CSA | Function | Template EC Number | Template Uniprot | Template Resolution |
|-------|---------|---------------------------------------|-----------------|---|------------|--------------------|------------------|---------------------|
| 1 | 0 | CYS 99 B;CYS 99 A;CYS 94 A;CYS 94 B | 3NOS | CYS 99 B;CYS 99 A;CYS 94 A;CYS 94 B | Structural | 1.14.13.39 | P29474 | 2.40 |
| 2 | 0.176 | CYS 99 B;CYS 94 A;CYS 99 A;CYS 94 B | 1PEG | CYS 306 A;CYS 244 A;CYS 313 A;CYS 308 A | Regulatory | 2.1.1.43 | P02303 | 2.59 |
| 3 | 0.231 | CYS 99 B;CYS 94 B;CYS 94 A;CYS 99 A | 3NOS | CYS 99 B;CYS 99 A;CYS 94 A;CYS 94 B | Structural | 1.14.13.39 | P29474 | 2.40 |
| 4 | 0.254 | CYS 99 B;CYS 99 A;CYS 94 B;CYS 94 A | 3NOS | CYS 99 B;CYS 99 A;CYS 94 A;CYS 94 B | Structural | 1.14.13.39 | P29474 | 2.40 |
| 5 | 0.273 | CYS 94 A;CYS 94 B;CYS 99 B;CYS 99 A | 3NOS | CYS 99 B;CYS 99 A;CYS 94 A;CYS 94 B | Structural | 1.14.13.39 | P29474 | 2.40 |
| 6 | 0.297 | CYS 94 A;CYS 99 B;CYS 99 A;CYS 94 B | 1PEG | CYS 306 A;CYS 244 A;CYS 313 A;CYS 308 A | Regulatory | 2.1.1.43 | P02303 | 2.59 |
| 7 | 0.297 | CYS 94 B;CYS 99 A;CYS 94 A;CYS 99 B | 1PEG | CYS 306 B;CYS 313 B;CYS 306 B;CYS 244 B | Regulatory | 2.1.1.43 | P02303 | 2.59 |
| 8 | 0.305 | CYS 94 A;CYS 99 B;CYS 94 B;CYS 99 A | 1PEG | CYS 306 A;CYS 244 A;CYS 313 A;CYS 308 A | Regulatory | 2.1.1.43 | P02303 | 2.59 |
| 9 | 0.316 | CYS 99 B;CYS 94 A;CYS 94 B;CYS 99 A | 1PEG | CYS 306 A;CYS 244 A;CYS 313 A;CYS 308 A | Regulatory | 2.1.1.43 | P02303 | 2.59 |
| 10 | 0.337 | CYS 94 B;CYS 99 B;CYS 94 A;CYS 99 A | 4XB6 | CYS 244 D;CYS 272 D;CYS 266 D;CYS 241 D | Structural | 4.7.1.1 | P16688 | 1.70 |

Showing 1 to 10 of 200 entries

← Previous 1 2 3 4 5 Next →

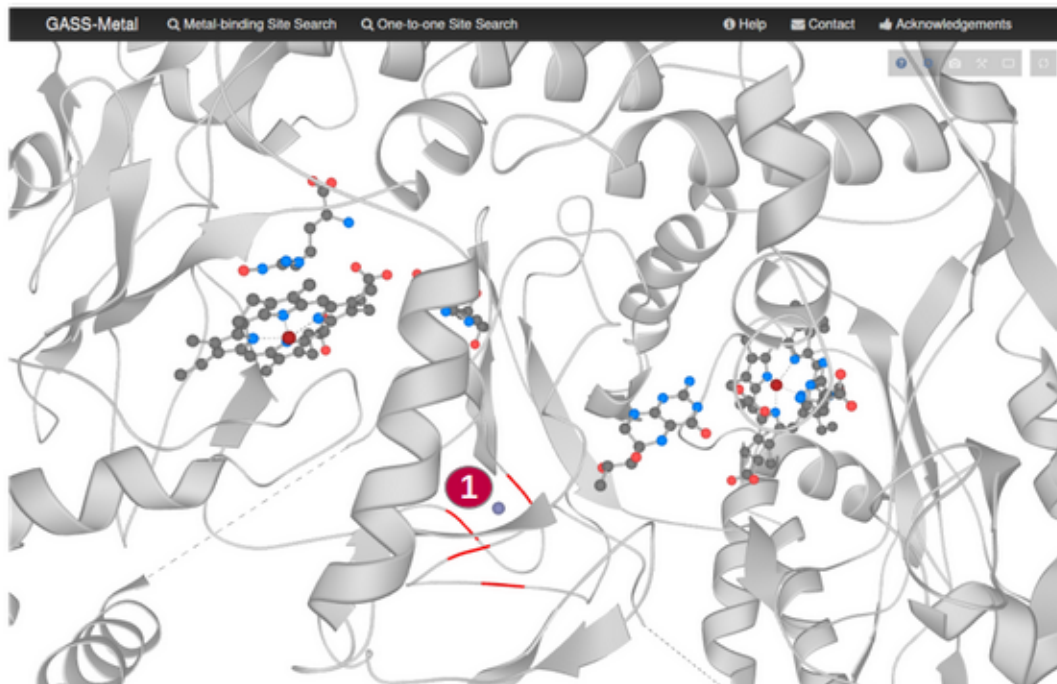
Run another search Download results **11**

Results

In **Metal-binding Site Search**, your results will be displayed in a table format with the following information:

- Shows or hides options and properties of templates **(1)**.
- Job ID **(2)** - can be used to retrieve the results later adding it to the webserver URL following the format:
`http://gassmetal.unifei.edu.br/prediction/csa_1633125413.45/mbs`
- Fitness score of matched residues **(3)**.
- Residues found by GASS-Metal on input structure matching a template **(4)**.
- PDB ID of a matched template **(5)**.
- Residues of matched template **(6)**.
- Function of the metal site **(7)**, EC Number **(8)**, Uniprot accession code **(9)** and Resolution **(10)** of a matched template.
- The results may also be downloaded as a CSV file **(11)**.
- The icon in the shape of an eye **(4 and 5)** opens the LiteMol Viewer.

LiteMol Viewer



The screenshot displays the LiteMol Viewer interface. At the top, there is a navigation bar with the following elements: "GASS-Metal", "Q Metal-binding Site Search", "Q One-to-one Site Search", "Help", "Contact", and "Acknowledgements". The main view shows a protein structure represented by grey ribbons, with a metal-binding site highlighted in red and labeled with a circled "1". Below the protein structure is a table with the following data:

| Index | Fitness | Found Active Site |
|-------|---------|-------------------------------------|
| 1 | 0 | CYS 99 B;CYS 99 A;CYS 94 A;CYS 94 B |
| 2 | 0.176 | CYS 99 B;CYS 94 A;CYS 99 A;CYS 94 B |
| 3 | 0.231 | CYS 99 B;CYS 94 B;CYS 94 A;CYS 99 A |
| 4 | 0.254 | CYS 99 B;CYS 99 A;CYS 94 B;CYS 94 A |
| 5 | 0.273 | CYS 94 A;CYS 94 B;CYS 99 B;CYS 99 A |
| 6 | 0.294 | CYS 94 A;CYS 99 B;CYS 99 A;CYS 94 B |

LiteMol Viewer

The amino acid residues found by GASS-Metal can be visualized through the icon in the shape of an eye in the result pages. This icon starts LiteMol and displays the amino acid residues found in red colour **(1)**.

The GASS-Metal results list is also available **(2)**.

One-to-one Site Search

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One-to-one Site Search

GASS-Metal

Step 1

Please provide a reference protein structure (PDB format):

Upload your own PDB file:

Choose PDB file

1

Provide a 4-letter PDB code or UniProt code (AlphaFold):

3NOS

Step 2

2

Please provide a template site:

HIS,99,A;HIS,94,B; HIS, 99, B

Use the following format for each residue:

Residue name, position on PDB, chain.

The information regarding a residue (i.e., 3-letter code, position on the sequence and chain ID) must be comma-separated (,) and each residue of the template must be separated by a semi-colon (;).

Example:
HIS,57,E; ASP,102,E; SER,195,E

Step 3

3

Please provide any residue mutation:

Use the following format:

Residue name, residue name.

If more than one mutation is needed, please separate the mutations using a semi-colon (;).

Example:
HIS,CYS;GLU,ASP;SER,HIS

Please select the reference atom:

4

Last heavy atom (LHA) of the si

Step 4

Please provide a target protein structure (PDB format):

Upload your own PDB File:

Choose PDB file

5

Or

Provide a 4-letter PDB code or UniProt code (AlphaFold):

3NSE

6 Run GASS

7 Run Example

Disclaimer: No PDB files will be retained on the system after being uploaded by the user.

How to run One-to-one Site Search

To perform a site search based on your own template:

- **Step 1:** Users must provide a 4-letter PDB code or UniProt code (AlphaFold), or provide a PDB file (1), which will serve as a reference for searching metal-binding sites by GASS-Metal.
- **Step 2:** Once the protein has been defined, it must be indicated what the reference template (which must be contained in the reference protein) on which the search will be based (2).
- **Step 3:** In this step, users can indicate whether to use conservative mutations or not (3). When choosing conservative mutations, inform which residues can be replaced in the target protein. Users can choose between alpha carbon or the last heavy atom (LHA) as the reference atom in the templates (4).
- **Step 4:** Users must provide a 4-letter PDB code or UniProt code (AlphaFold), or provide a PDB file (5), which will serve as a target for searching metal-binding sites. It is in this protein that GASS-Metal will search for sites similar to the template informed in step 2.

Finally, click on the button **Run GASS (6)** to perform the search.

The button **Run Example (7)** will perform a metal-binding site search based on a pre-defined example.