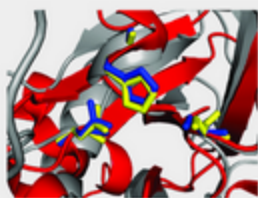


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GASS



Genetic Active Site Search

GASS-WEB: a web server for identifying enzyme active sites based on genetic algorithms

Sandro C. Izidoro*, Douglas E. V. Pires*, Raquel C. de Melo-Minardi, Gisele L. Pappa

Abstract

Structure-guided methods have been proposed over the years to infer protein function based on active site similarity. Given an active site template, these methods use different mathematical modelling and searching procedures to match the template to a given set of proteins. Many of the current available methods present, however, limitations such as performing only exact matches on template residues (not accounting for conservative changes), pruning the search space using ad-hoc procedures, besides finding inter-domain active sites. In order to tackle these problems, we have recently proposed GASS (Genetic Active Site Search), a search method based on genetic algorithms that aims to cope with the aforementioned issues. Here we propose a user-friendly web server implementing the method's capabilities, called GASS-WEB.

GASS-WEB can be used under two different scenarios: (a) given a protein of interest, to try to match a set of specific templates (i.e., known active sites); or (b) given an active site template, looking for it in a database of protein structures.

The method has shown to be very effective on a range of experiments. Based on the Catalytic Site Atlas (CSA) annotation, it was able to correctly identify >90% of the catalogued active sites. It also managed to achieve a MCC of 0.63 on the CASP 10 data set (ranking fourth among 18 methods).

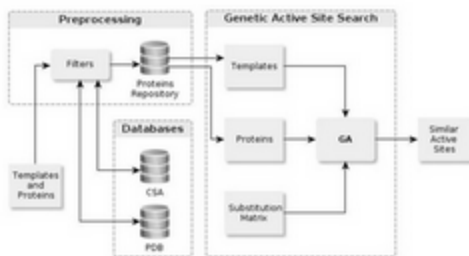
Available Resources

CSA
templates

Performs active site search using literature-derived and PSI-BLAST templates from CSA, given a PDB file.

NCBI-VAST
database

Performs active site search using a user-provided template on the NCBI-VAST database.



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About GASS

GASS-WEB is a user-friendly web server for active site search based on genetic algorithms. It can be used under two different scenarios:

- **CSA Site Search (1):** Given a protein of interest, try to match a set of specific templates (i.e., known active sites) annotated at the Catalytic Site Atlas (CSA).
- **NCBI Template Search (2):** Given an active site template provided by the user, look for it in a database of protein structures derived from the NCBI-VAST data set.

Submission page

How to run GASS-WEB

GASS CSA Site Search NCBI Template Search

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Site Search Based on the Catalytic Site Atlas



Genetic Active Site Search

Run example

Disclaimer

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

Step 1: Please provide a protein structure (PDB format)

Description

Upload your own PDB file:

No file selected.

2

Provide a 4-letter PDB code:

Step 2: Please select a template size

Description

Select template size (number of residues)

3

4

U F *m* G

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To perform a site search based on the list of templates from the Catalytic Site Atlas:

- Click on "CSA Site Search" (1) to open the submission page.
- Provide the protein structure by either uploading your own file (2), which must comply with the PDB format, or supplying a 4-letter PDB code.
- The next step is to choose the template size for matching (3), which is the number of residues of the active site.
- You are then ready to submit your query to GASS-WEB (4).

Results page

GASS CSA Site Search NCBI Template Search

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Visualization controls

Show template properties

Predicted active sites

Job-ID: csa_1419852614.76

10 records per page

Search:

Index	Fitness	Found active site on query PDB	Template PDB ID	Matched template on CSA	Template EC Number	Template Uniprot	Template Resolution
1	1.84	HIS 57 A;ASP 113 A;SER 194 A;GLY 195 A	1N8O	HIS 57 B;ASP 102 B;SER 195 C;GLY 196 C	3.4.21.1	P23827	2.00
2	2.92	HIS 57 A;ASP 113 A;SER 194 A;GLY 211 A	1N8O	HIS 57 B;ASP 102 B;SER 195 C;GLY 196 C	3.4.21.1	P23827	2.00
3	2.92	CYS 6 A;GLY 187 A;HIS 148 A;CYS 216 A	1MEK	CYS 36 A;GLY 37 A;HIS 38 A;CYS 39 A	5.3.4.1	P07237	NOT
4	3.14	HIS 57 A;ASP 113 A;GLY 192 A;SER 194 A	1HJA	HIS 57 B;ASP 102 B;GLY 193 C;SER 195 C	3.4.21.1	P68390	2.30
5	3.18	ASP 113 A;SER 5 A;ARG 156 A;ASN 77 A	1C17	ASP 61 A;SER 206 M;ARG 210 M;ASN 214 M	NULL	P0AB98	NOT
6	4.08	CYS 216 A;GLY 4 A;HIS 148 A;CYS 6 A	1MEK	CYS 36 A;GLY 37 A;HIS 38 A;CYS 39 A	5.3.4.1	P07237	NOT
7	4.61	CYS 216 A;SER 5 A;CYS 6 A;ARG 223 A	1AHJ	CYS 113 C;SER 114 C;CYS 115 C;ARG 56 D	4.2.1.84	P13449	2.65
8	4.81	HIS 57 A;ASP 113 A;GLY 212 A;SER 194 A	1HJA	HIS 57 B;ASP 102 B;GLY 193 C;SER 195 C	3.4.21.1	P68390	2.30
9	5.2	SER 158 A;HIS 148 A;HIS 149 A;ASP 9 A	1AJ8	SER 193 A;HIS 223 A;HIS 262 A;ASP 312 A	4.1.3.7	Q53554	1.90
10	5.6	CYS 216 A;SER 5 A;CYS 6 A;ARG 223 A	1AHJ	CYS 113 A;SER 114 A;CYS 115 A;ARG 56 B	4.2.1.84	P13449	2.65

Showing 1 to 10 of 200 entries

← Previous 1 2 3 4 5 Next →

Run another search

Download results

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Results

For a **CSA Site Search** query, your results will be displayed in a table format with the following information:

- Job ID - which can be used by the user to retrieve the results later (1), by adding it to the web server URL following the format: *http://gassweb.dcc.ufmg.br/prediction/job_id*
- Fitness score of matched residues - modified RMSD (2).
- List of residues found by GASS-WEB on input structure matching a template (3).
- PDB ID of matched template (4).
- Residue list of matched template (5).
- EC Number (6), Uniprot accession code (7) and resolution (8) of matched template.

The results may also be downloaded as a tab-separated file (9).

Contact page

Getting in touch



Contact

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In case you experience any trouble using GASS-WEB or have any suggestions or comments, please do not hesitate in contacting us **(1)** either via e-mail or through the online form.