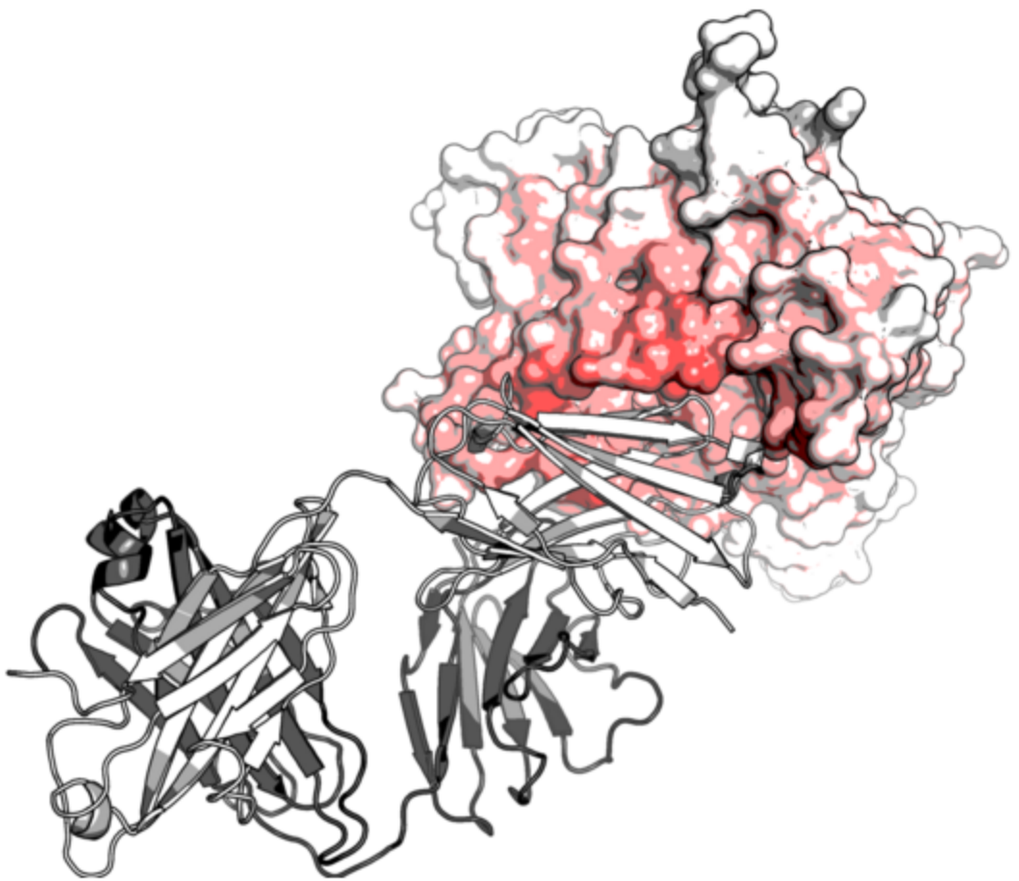
mCSM-AB

mCSM-AB: a web server for predicting antibody-antigen affinity changes upon mutation with graph-based signatures

Douglas E. V. Pires & David B. Ascher



Abstract

Summary: Computational methods have traditionally struggled to predict the effect of mutations in antibody-antigen complexes on binding affinity. This has limited their usefulness during antibody engineering and development, and their ability to predict biologically relevant escape mutations. Here we demonstrate that graph-based signatures can be used to accurately predict the effect of mutations on antibody binding affinity. We show that mCSM-AB performs better than comparable methods that have been previously used for antibody engineering.

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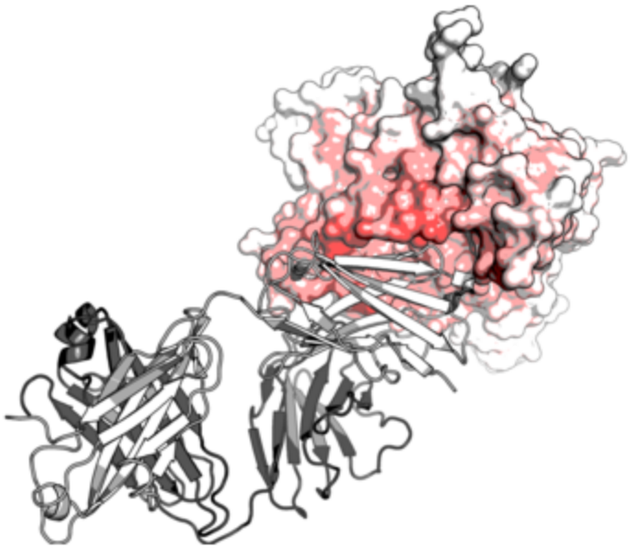
Antibody-Antigen Affinity Changes Upon Mutation



Run example

Disclaimer

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

Single mutation

Description

Wild-type AB complex - PDB format (Ex.: 3NGB)

Choose file No file chosen

Mutation (Example: G54S)

Mutation chain (Example: H)

▶Run regression

2

Mutation list

Description

Wild-type AB complex - PDB format (Ex.: 3NGB)

Choose file No file chosen

3

Mutation list file Format

Choose file No file chosen

4

▶Run regression

Antibody-Antigen Affinity Change Upon Mutation

Predicted Affinity Change (ΔΔG):

-1.336 Kcal/mol (*Reduced affinity*)

1

Mutation:

2

Wild-type: **GLY**
Position: **54**
Mutant-type: **SER**
Chain: **H**

Run another prediction

Molecule Visualization

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Antibody-Antigen Affinity Change Upon Mutation

Predicted Affinity Change (ΔΔG):

10 records per page

1 2 3 4

Index	PDB File	Chain	Wild Residue	Residue Position	Mutant Residue	RSA (%)	Predicted ΔΔG	Outcome
11	3NGB.pdb	B	T	70	Y	70.5	0.36	Increased affinity
12	3NGB.pdb	D	G	471	N	19.6	-0.912	Reduced affinity
13	3NGB.pdb	G	T	406	V	62.4	-0.055	Reduced affinity
14	3NGB.pdb	H	M	69	F	0.1	-0.464	Reduced affinity
15	3NGB.pdb	F	D	187	M	56.0	-0.529	Reduced affinity
16	3NGB.pdb	K	L	78	K	1.1	-0.281	Reduced affinity
17	3NGB.pdb	J	H	102	D	25.8	-0.624	Reduced affinity
18	3NGB.pdb	A	T	63	C	90.2	-0.522	Reduced affinity
19	3NGB.pdb	G	K	207	L	41.3	0.072	Increased affinity
20	3NGB.pdb	B	G	65	M	120.1	-0.57	Reduced affinity

Showing 11 to 20 of 30 entries

← Previous 1 2 3 Next →

Run another prediction | Download results

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