 **HawkDock** <http://cadd.zju.edu.cn/hawkdock/>
A web server for the structural prediction and analysis of protein-protein complex.

HawkDock MM/GBSA **Make sure you are on this tab.**

MM/GBSA is employed to predict the **binding free energy** and **decompose** the free energy contributions to the binding free energy of a protein-protein complex in per-residue to help you analyze the binding structures.

Warning! Please check the **Help** when you first use MM/GBSA.

Job Name (optional)

Email (optional)

Input Complex C_re...st.pdb

Chain ID of Receptor

Chain ID of Ligand

ABSOLUTELY complete this step. The queue is long & you will want to be notified when your job is completed.

Enter chain IDs of citrate synthase separated by semicolon, no spaces

Enter chain IDs of malate dehydrogenase separated by semicolon, no spaces

Example of PDB File: [Complex](#) / [Chain ID of Receptor](#) / [Chain ID of Ligand](#) / [Result](#)
Example of PDB ID: [Complex](#) / [Chain ID of Receptor](#) / [Chain ID of Ligand](#) / [Result](#)

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Results for job: CS_A_MDH_C

Status of your job: **Waiting.**

Estimated time: **Estimate the run time when the job starts running.**

Submitted time: 2021-09-16 06:18 (UTC + 8 hours).


Start time: Unknown.

Step 0: Queue in cluster system.
Step 1: Tleap.
Step 2: Minimization.
Step 3: MM/GBSA.
Step 4: Finished.

You can check the **queue** to learn more about the status of your job.
This page will update every 20 seconds until finished.
You can **bookmark this page** to get your results later.
If you have provided a valid email address, an email will be sent to you with a link to the results page when your job is finished.
The results will be kept on the server for two weeks.

Screen you will see after submitting your job. You can bookmark this page and check status of run.

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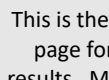
[Home](#) [Help](#) [Queue](#) [Papers](#) [Contact](#)

No.	Job name	Type	Status	Submitted time
71366	S3_40	MM/GBSA	Waiting	2021-09-19 03:09:28 (UTC + 8 hours)
71365	S3_39	MM/GBSA	Waiting	2021-09-19 03:08:49 (UTC + 8 hours)
71364	S3_38	MM/GBSA	Waiting	2021-09-19 03:08:16 (UTC + 8 hours)
71363	S3_37	MM/GBSA	Waiting	2021-09-19 03:07:51 (UTC + 8 hours)
71362	S3_36	MM/GBSA	Waiting	2021-09-19 03:07:30 (UTC + 8 hours)
71361	S3_35	MM/GBSA	Waiting	2021-09-19 03:06:49 (UTC + 8 hours)
71360	S3_34	MM/GBSA	Waiting	2021-09-19 03:06:24 (UTC + 8 hours)
71359	S3_33	MM/GBSA	Waiting	2021-09-19 03:06:02 (UTC + 8 hours)
71358	S3_32	MM/GBSA	Waiting	2021-09-19 03:05:24 (UTC + 8 hours)
71357	S3_31	MM/GBSA	Waiting	2021-09-19 03:05:01 (UTC + 8 hours)
71356	S3_30	MM/GBSA	Waiting	2021-09-19 03:04:38 (UTC + 8 hours)
71355	S3_29	MM/GBSA	Waiting	2021-09-19 03:04:14 (UTC + 8 hours)
71354	S3_28	MM/GBSA	Waiting	2021-09-19 03:03:44 (UTC + 8 hours)
71353	S3_27	MM/GBSA	Waiting	2021-09-19 03:03:21 (UTC + 8 hours)
71352	S3_26	MM/GBSA	Waiting	2021-09-19 03:02:14 (UTC + 8 hours)
71351	imp	MM/GBSA	Waiting	2021-09-19 02:56:06 (UTC + 8 hours)
71350	S3_25	MM/GBSA	Waiting	2021-09-19 02:52:00 (UTC + 8 hours)
71349	S3_24	MM/GBSA	Waiting	2021-09-19 02:51:41 (UTC + 8 hours)
71348	S3_23	MM/GBSA	Waiting	2021-09-19 02:51:19 (UTC + 8 hours)
71347	S3_22	MM/GBSA	Waiting	2021-09-19 02:50:53 (UTC + 8 hours)

No.	Job name	Type	Status	Submitted time
70804	sp92	HawkDock	Waiting	2021-09-16 13:44:08 (UTC + 8 hours)
70803	sp87	HawkDock	Waiting	2021-09-16 13:43:52 (UTC + 8 hours)
70802	sp85	HawkDock	Waiting	2021-09-16 13:43:40 (UTC + 8 hours)
70801	sp84	HawkDock	Waiting	2021-09-16 13:43:24 (UTC + 8 hours)
70800	sp81	HawkDock	Waiting	2021-09-16 13:43:11 (UTC + 8 hours)
70799	sp80	HawkDock	Waiting	2021-09-16 13:42:52 (UTC + 8 hours)
70798	sp79	HawkDock	Waiting	2021-09-16 13:42:37 (UTC + 8 hours)
70797	sp78	HawkDock	Waiting	2021-09-16 13:42:21 (UTC + 8 hours)
70796	sp75	HawkDock	Waiting	2021-09-16 13:42:05 (UTC + 8 hours)
70795	sp72	HawkDock	Waiting	2021-09-16 13:41:45 (UTC + 8 hours)
70794	sp71	HawkDock	Waiting	2021-09-16 13:40:50 (UTC + 8 hours)
70793	sp69	HawkDock	Waiting	2021-09-16 13:40:33 (UTC + 8 hours)
70792	sp68	HawkDock	Waiting	2021-09-16 13:40:18 (UTC + 8 hours)
70791	sp67	HawkDock	Waiting	2021-09-16 13:40:04 (UTC + 8 hours)
70790	sp64	HawkDock	Waiting	2021-09-16 13:39:49 (UTC + 8 hours)
70789	sp61	HawkDock	Waiting	2021-09-16 13:39:32 (UTC + 8 hours)
70788	sp62	HawkDock	Waiting	2021-09-16 13:39:01 (UTC + 8 hours)
70787	sp60	HawkDock	Running	2021-09-16 13:38:53 (UTC + 8 hours)
70786	ID501338	MM/GBSA	Running	2021-09-16 13:17:40 (UTC + 8 hours)
70785	gammat	MM/GBSA	Completed	2021-09-16 12:48:45 (UTC + 8 hours)

You can see where you are in the queue of jobs. Find your job listed and then find the job that is actually running.

Your job will be on page 1; In this example, the job running is on page 10 (~200 jobs in front of your job!). Each job runs for ~1-2 h.



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Results

Results for job: CS_A_MDH_C

Binding free energy of complex: **-44.65** (kcal/mol)

Downloadable Files:

[CS_A_MDH_C-1631744298277.csv](#)

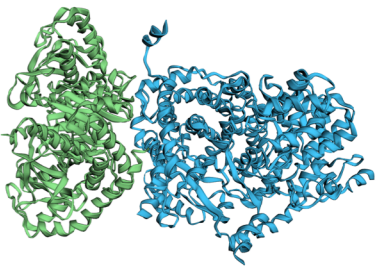
[Receptor PDB File](#)

[Ligand PDB File](#)

Rank	Residue (Rec)	Binding Free Energy
1	B-GLN-100	-4.76
2	B-THR-23	-4.57
3	B-TYR-69	-3.76
4	A-ILE-431	-2.93
5	B-GLU-104	-2.75

Showing 1 to 5 of 902 rows

Molecule visualization



Action Options:

- Rotate: Press and hold the left mouse button.
- Zoom: Use mouse's scroll button.
- Translate: Press and hold mouse's scroll button.

Browsers Requirements

Please make sure that WebGL is enabled in your browser. To test for WebGL support, see <http://webglreport.com/?v=1>.

- Support: Chrome, Firefox (version 4 or later), Safari, Microsoft Edge, Internet Explorer (version 11).

This is the landing page for your results. Make sure to download your .csv file of results.

If you check the boxes, these residues will be highlighted in red so that you can see their location on the structure

http://cadd.zju.edu.cn/hawkdock/gbsa/CS_A_MDH_C-1631744298277

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This is an example of the .csv output file. The first row entry below the column titles is the total free energies of binding between “receptor” and “ligand” for each the energy components (VDW, ELE, GB, SA) and the total. The remainder of the file is the free energy of receptor/ligand binding on a per residue basis. You will have a list of residues in column 1.

1	RESIDUE_ID	VDW	ELE	GB	SA	TOTAL
2	lig-rec	-164.97	-166.22	305.45	-19.1	-44.85
3	R-A-ASP--7	0	0.01	-0.01	0	0
4	R-A-TYR--6	0	0	0	0	0
5	R-A-LYS--5	0	0.24	-0.24	0	0
6	R-A-ASP--4	0	-0.19	0.18	0	0
7	R-A-ASP--3	0	-0.17	0.17	0	0
8	R-A-ASP--2	0	-0.23	0.23	0	0
9	R-A-ASP--1	0	-0.24	0.24	0	0
10	R-A-LYS-0	0	0.17	-0.17	0	0
11	R-A-ALA-1	0	0	0	0	0
12	R-A-SER-2	0	0	0	0	0
13	R-A-SER-3	0	0.01	-0.01	0	0
14	R-A-THR-4	0	0.01	-0.01	0	0
15	R-A-ASN-5	0	0	-0.01	0	0
16	R-A-LEU-6	0	0	0	0	0
17	R-A-LYS-7	0	0.59	-0.59	0	0.01
18	R-A-ASP-8	0	-0.45	0.44	0	-0.01
19	R-A-ILE-9	0	-0.01	0.01	0	0

Compared with thermodynamic integration (TI) and free energy perturbation (FEP) approaches, the MM/PBSA and MM/GBSA approaches are more computationally efficient and allow for the decomposition into different interaction terms.^{27,29,30} In the spirit of MM/PBSA or MM/GBSA, the binding free energy

for a protein–protein complex can be calculated using the following equations:

$$\Delta G_{\text{bind}} = G_{\text{com}} - (G_{\text{rec}} + G_{\text{lig}}) \quad (1)$$

$$\Delta G_{\text{bind}} = \Delta H - T\Delta S \approx \Delta E_{\text{MM}} + \Delta G_{\text{sol}} - T\Delta S \quad (2)$$

$$\Delta E_{\text{MM}} = \Delta E_{\text{internal}} + \Delta E_{\text{electrostatic}} + \Delta E_{\text{vdw}} \quad (3)$$

$$\Delta G_{\text{sol}} = \Delta G_{\text{PB/GB}} + \Delta G_{\text{SA}} \quad (4)$$

where ΔG_{bind} represents the total binding free energy upon protein–protein binding; ΔE_{MM} is the total gas phase energy (sum of $\Delta E_{\text{internal}}$, $\Delta E_{\text{electrostatic}}$, and ΔE_{vdw}); ΔG_{sol} is the sum of polar ($\Delta G_{\text{PB/GB}}$) and non-polar (ΔG_{SA}) contributions to solvation; and $-T\Delta S$ is the conformational entropy upon binding (usually calculated by normal-mode analysis). $\Delta E_{\text{internal}}$ is the internal energy arising from the bond, angle, and dihedral terms in the molecular mechanics (MM) force field (this term always amounts to zero in the MM/PBSA and MM/GBSA calculations based on the single trajectory of a complex). $\Delta E_{\text{electrostatic}}$ and ΔE_{vdw} are the electrostatic and van der Waals energies from MM calculations. $\Delta G_{\text{PB/GB}}$ is the polar contribution to the solvation free energy (calculated *via* the Poisson–Boltzmann (PB) or generalized Born (GB) method). ΔG_{SA} is the nonpolar solvation free energy, usually computed with a linear function of the solvent-accessible surface area (SASA). MM/GBSA and MM/PBSA have been successfully applied to predict the binding free energies for various protein–protein/peptide complexes^{31–34} or identify the hot-spots at protein–protein binding interfaces,^{35–37} but the previous studies mostly focused on certain specific systems and the prediction results cannot afford the overall accuracy of MM/PBSA and MM/GBSA for protein–protein systems.



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Assessing the performance of the MM/PBSA and MM/GBSA methods. 6. Capability to predict protein–protein binding free energies and re-rank binding poses generated by protein–protein docking†

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This information on the free energy of binding terms is excerpted from the Chen et al. paper cited.