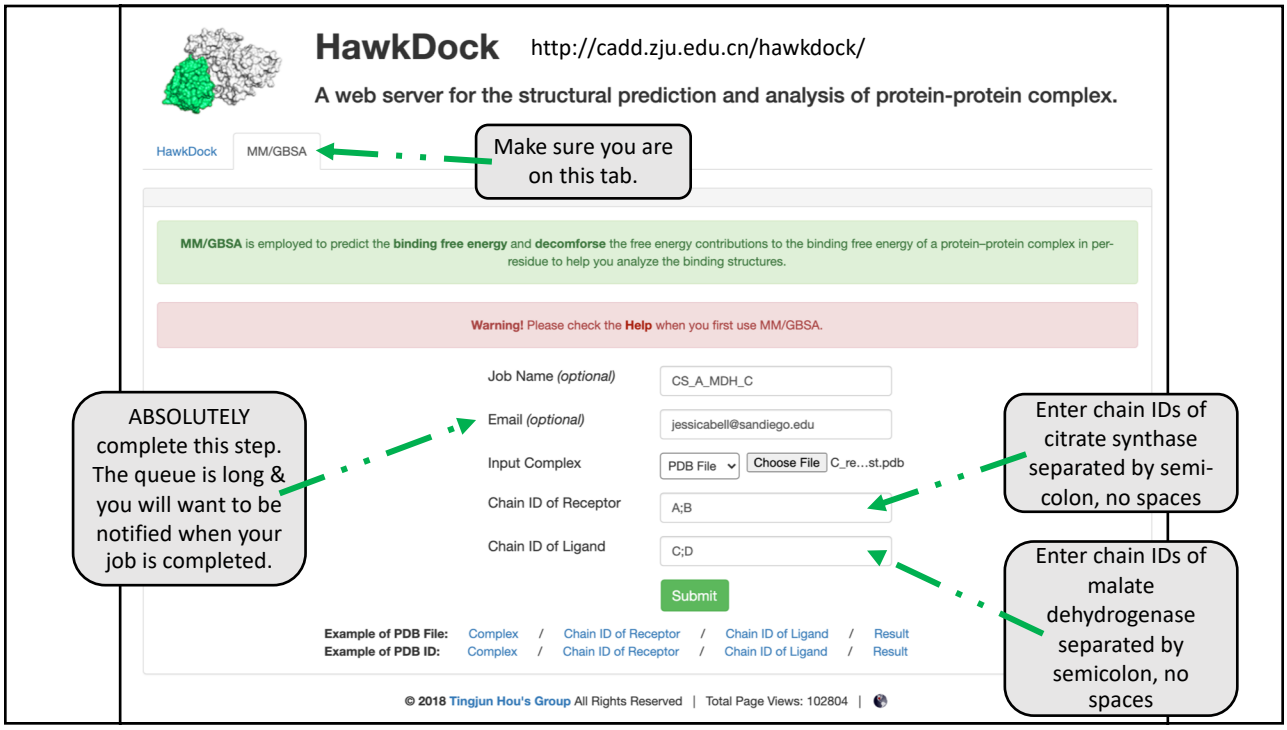
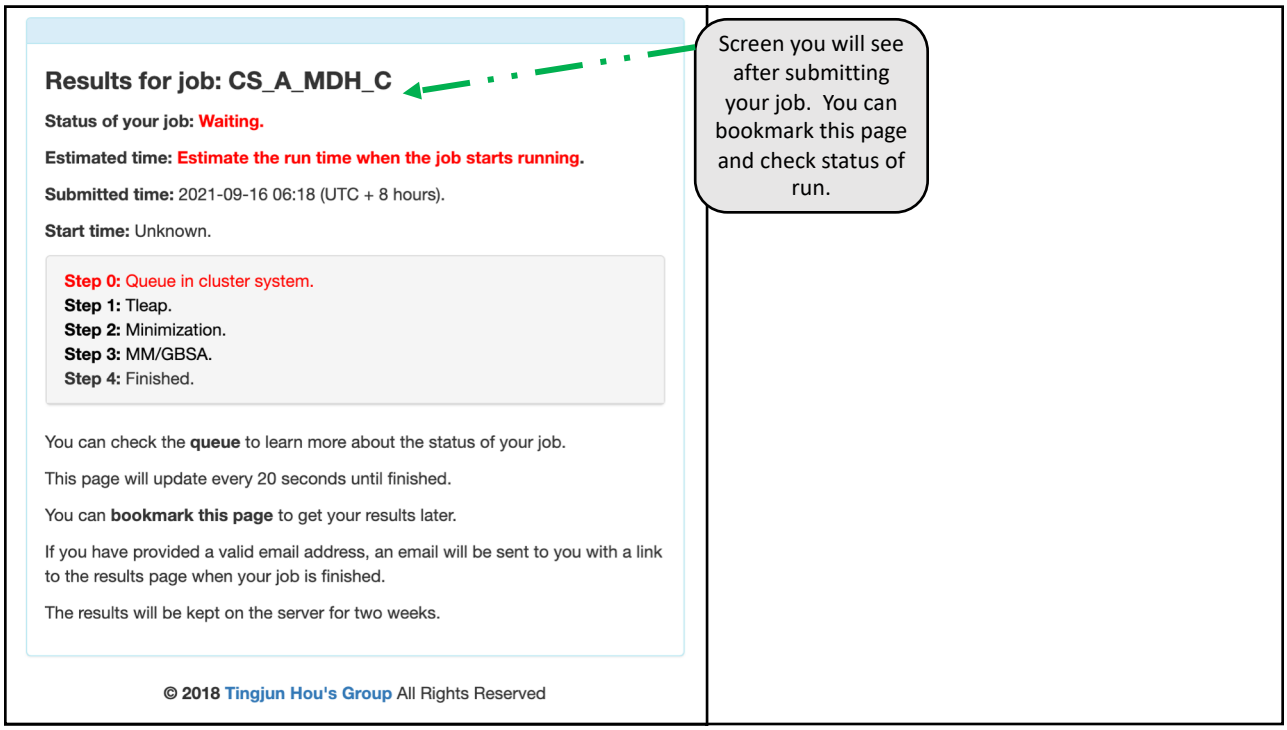
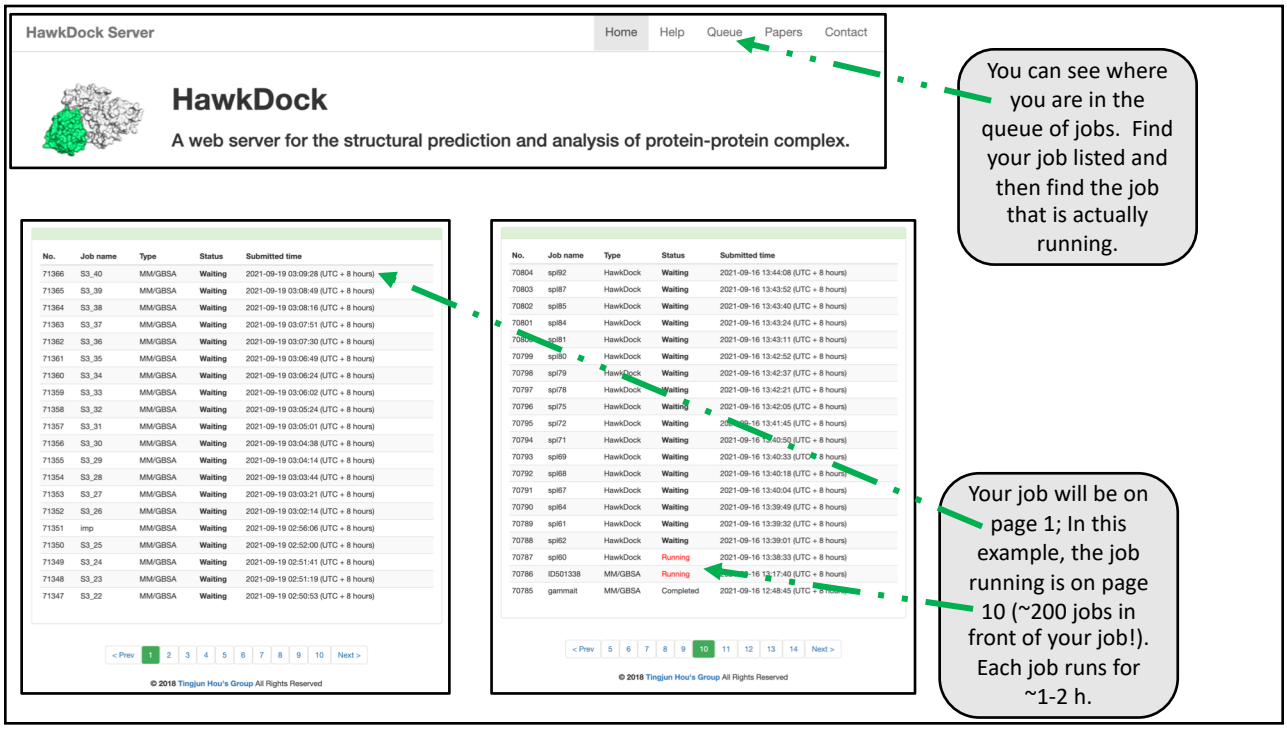

HawkDock
http://cadd.zju.edu.cn/hawkdock/
A web server for the structural prediction and analysis of protein-protein complex.
HawkDock
MM/GBSA
Make sure you are on this tab.
MM/GBSA is employed to predict the binding free energy and decomforse the free energy contributions to the binding free energy 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)
CS_A_MDH_C
Email (optional)
jessicabell@sandiego.edu
Input Complex
PDB File
Choose File
C_re...st.pdb
Chain ID of Receptor
A;B
Chain ID of Ligand
C;D
Submit
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
© 2018 Tingjun Hou's Group All Rights Reserved | Total Page Views: 102804 |
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 semi-colon, no spaces
Enter chain IDs of malate dehydrogenase separated by semicolon, no spaces


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.
© 2018 Tingjun Hou's Group All Rights Reserved
Screen you will see after submitting your job. You can bookmark this page and check status of run.


HawkDock Server
Home
Help
Queue
Papers
Contact
HawkDock
A web server for the structural prediction and analysis of protein-protein complex.
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.


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
HawkDock Server
Home
Help
Queue
Papers
Contact
Results
Results for job: CS_A_MDH_C
Binding free energy of complex: -44.85 (kcal/mol)
Downloadable Files:
CS_A_MDH_C-1631744298277.csv
Receptor PDB File
Ligand PDB File
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
Support: Chrome, Firefox (version 4 or later), Safari, Microsoft Edge, Internet Explorer (version 11).
http://cadd.zju.edu.cn/hawkdock/gbsa/CS_A_MDH_C-1631744298277

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.

	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.

CrossMark click for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2016, 18, 22129

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†

Fu Chen,[a] Hui Liu,[a] Huiyong Sun,[a] Peichen Pan,[a] Youyong Li,[c] Dan Li[a] and Tingjun Hou*[ab]

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