

Gaussian Job Submission

Gaussian job submission is performed in the following two steps:

1. **Data Preparation:** Set up the working directory and prepare input files
2. **Gaussian Settings:** Select/edit input, configure computational resources, and submit the job

You can switch between these steps using the tabs at the top of the screen.

Data Preparation

Please refer to the [corresponding page](#).

Gaussian Settings


Input File Configuration

? File Selection

- Selection Method: Use the "Browse" button to open the file browser, or enter the file path directly
- Preview Function: The contents of the file will be displayed automatically after selection

? File Editing

- Integrated Editor: Click the "Edit" button to directly edit the input file
- Save: Click the "Save" button to save changes

 **Input File**

Gaussian Input File

Path to the Gaussian input file (.com or .gjf)

```
#p rb3lyp/3-21g force test scf=novaracc

Gaussian Test Job 397:
Valinomycin force2

0,1
0,-1.3754834437,-2.5956821046,3.7664927822
0,-0.3728418073,-0.530460483,3.8840401686
```

Script Editor test0397.com

```
1 #p rb31yp/3-21g force test scf=nowaracc
2
3 Gaussian Test Job 397:
4 Valinomycin force2
5
6 0,1
7 0,-1.3754834437,-2.5956821046,3.7664927822
8 0,-0.3728418073,-0.530460483,3.8840401686
9 0,2.3301890394,0.5231526187,1.7996834334
10 0,0.2842272248,2.5136416005,-0.2483875054
11 0,2.3870396194,3.3004808604,0.2860546915
12 0,3.927241841,1.9677029583,-2.7261655162
13 0,2.2191878407,-1.0673859692,-2.0338343532
14 0,4.209257915,-1.2459024314,-3.1616013359
15 0,1.7622263124,-1.2194205092,-5.8516071343
16 0,1.0363626567,3.1095923678,-3.7084594295
17 0,0.2486786219,0.966590651,-3.8828785542
18 0,-2.5586288262,-0.0906355161,-1.9360823389
19 0,-0.3281133832,-2.3890727819,0.2344263336
```

Cancel Save

Gaussian Version Selection


? Available Versions

Gaussian 16, Gaussian 09

? G16 Revision Selection

When Gaussian 16 is selected, choose from the following revisions:

c02, c01, b01

 Gaussian Version

Gaussian 16

Gaussian 09

G16 Revision

g16c02 (C.02) ▼

Select the revision of Gaussian 16.

Computational Resource Settings

? Job Type Selection

Standard Computation

- 1–64 or 128 cores

Large-Memory Computation

- Use when standard memory is insufficient.
- Only 64 or 128 cores can be selected.

GPU Computation

- Not recommended due to limited speedup.
- Maximum 16 cores per GPU, up to a total of 128 cores.

? CPU Core Count Setting

- Preset Selection: 1, 4, 8, 16, 32, 64, or 128 cores
- Manual Input: Enter any desired core count in the input field

? GPU Settings (when GPU computation is selected): Set from 1 to 8 units

? Wall Time Setting: Specify individually in hours, minutes, and seconds

? Storage Options

- Use the high-capacity /gwork directory as a scratch area
- Slightly slower performance

Resource Settings

Job Type

Standard Computation

Standard Gaussian computation

CPU Cores

1

4

8

16

32

64

128

8

Select a value between 1 and 64, or 128

Maximum Execution Time

72

0

0

Hours

Minutes

Seconds

☐ Use large scratch area

Use a slower but larger capacity scratch area.
Suitable for large-scale calculations.

⚙️ Advanced Settings

▼

Advanced Settings (Optional)



Click "Advanced Settings" to expand and configure the following options:

? Notification Settings: **Receive email notifications when the job starts and finishes**

? Overwrite Existing Files: **Set behavior when files with the same name already exist**

? Job Name Settings:

- Enter a custom job name
- If left blank, a name will be auto-generated from the input file
(e.g., test0397.com → test0397)

 Advanced Settings 

☐ Send email notifications

Receive email notifications when the job starts and ends

☐ Overwrite existing files

Overwrite files that already exist with the same name


Job Name (optional)

Will be auto-generated from input file if


Name used to identify the job (can be omitted)

Job Submission

Click the "Submit Job" button

 Job Submission

The Gaussian job will be submitted with the settings above. Please click the 'Submit Job' button if everything is correct.

 Submit Job