# **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	~/ccood_job/tes	Browse	🖉 Edit			
		Path to the Gaussian i	nput file (.com o	r .gjf)			
<pre>#p rb3lyp/3-21g force test scf=novaracc</pre>							
							Gaussian Test Job 397:
	Valinomycin force2						
	0,1 0 -1 3754834437 -2 5956821046 3 7664927822						
	0,-1.3754834437	,-2.5956821046,3.76	564927822				
	0,-1.3754834437 0,-0.3728418073	,-2.5956821046,3.70 ,-0.530460483,3.884	564927822 10401686				
	0,-1.3754834437 0,-0.3728418073	,-2.5956821046,3.70 ,-0.530460483,3.884	564927822 10401686				
	0,-1.3754834437 0,-0.3728418073	,-2.5956821046,3.70 ,-0.530460483,3.884	564927822 40401686 ×	test0397.co			
1	0,-1.3754834437 0,-0.3728418073	,-2.5956821046,3.70	564927822 40401686 ×	test0397.co			
1 2 3	0,-1.3754834437 0,-0.3728418073 prb3lyp/3-21g force test scf=novarace Gaussian Test Job 397:	,-2.5956821046,3.70	564927822 40401686 ×	test0397.co			
1 2 3 4 5	0,-1.3754834437 0,-0.3728418073	,-2.5956821046,3.70	564927822 10401686 ×	test0397.com			
1 2 3 4 5 6	0,-1.3754834437 0,-0.3728418073	,-2.5956821046,3.70	564927822 10401686 ×	test0397.com			
1 2 3 4 5 6 7	0,-1.3754834437 0,-0.3728418073	,-2.5956821046,3.76 ,-0.530460483,3.884	564927822 40401686 ×	test0397.co			
1 2 3 4 5 6 7 8 9	0,-1.3754834437 0,-0.3728418073 p rb31yp/3-21g force test scf=novarace Gaussian Test Job 397: Valinomycin force2 e,1 0,-1.3754834437,-2.5956821046,3.7664927 0,-0.3728418073,-0.5956821046,3.7664927 0,-0.3728418073,-0.59568210465,3.7664927 0,-0.3728418073,-0.59568210465,3.7664927	,-2.5956821046,3.76 ,-0.530460483,3.884	564927822 40401686 ×	test0397.co			
1 2 3 4 5 6 7 8 9 9	0,-1.3754834437 0,-0.3728418073 %p rb3lyp/3-21g force test scf=novaracc Gaussian Test Job 397: Valinomycin force2 0,1 0,-1.3754834437,-2.5956821046,3.7664927 0,-2.37548390394,0.5231526187,1.79683433 0,2.381890394,0.5231526187,1.79683433	,-2.5956821046,3.76 ,-0.530460483,3.884	564927822 40401686 ×	test0397.co			
1 2 3 4 5 6 7 8 9 9 10 11	0,-1.3754834437 0,-0.3728418073 %p rb3lyp/3-21g force test scf=novaracc Gaussian Test Job 397: Valinomycin force2 0,-1.3754834437,-2.5956821046,3.7664927 0,-1.3754834437,-2.5956821046,3.7664927 0,-2.381890394,0.531520187,1.79963433 0,0.284128228,2.513641685,-0.2483875 0,2.8870396134,3.30448866,0.286554697	,-2.5956821046,3.76 ,-0.530460483,3.884 	564927822 40401686 ×	test0397.co			
1 2 3 4 5 6 7 8 9 10 11 12 13	0,-1.3754834437 0,-0.3728418073 ////////////////////////////////////	, -2.5956821046, 3.76 , -0.530460483, 3.884	564927822 10401686 ×	test0397.co			
1 2 3 4 5 6 7 8 9 10 11 12 13 14	O, -1.3754834437 O, -0.3728418073 b, -0.3728418073 b, -0.3728418073 b, -0.3728418073 b, -0.3728418073 b, -1.37483437, -2.5956821046, 3.7664927 0, -3.73483437, -2.5956821046, 3.7664927 0, -3.734834437, -2.5956821046, 3.7664923 0, -3.2741841, 3.50416084, -3.8640401 0, -3.2741841, 3.50416084, -3.8640401 0, -3.2741841, 3.50416084, -3.8640401 0, -3.2741841, 1.5677029583, -2.763518 0, -3.2741841, 1.5677029583, -2.763518 0, -3.2741841, 1.5677029583, -2.763518 0, -3.2957915, -1.2459024314, -3.16160133 0, -3.2957915, -1.2459024314, -3.16160133	, -2.5956821046, 3.76 , -0.530460483, 3.884	564927822 10401686 × Concentra	test0397.co			
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	0,-1.3754834437 0,-0.3728418073 prb3]yp/3-21g force test scf=novarace Gaussian Test Job 397: Vallnemycin force2 0,1 0,-1.3754834437,-2.9556821046,3.7654927 0,-0.3728418073,-0.533460483,3.8849401 0,-3.38189834,0.53315614685,-0.24838756 0,2.38198364,3.30048886,0.28685640 0,3.97241841,1.96782988,-2.76615515 0,2.3819878407,-1.69782988,-2.76615515 0,2.3819878407,-1.697829883,-2.76615515 0,2.391978407,-1.269782443,-3.581607 0,1.0858265767,3.109922987,-1.7988343 0,1.0858265767,3.109922987,-1.79898434	, -2.5956821046, 3.76 , -0.530460483, 3.884	564927822 40401686 × concentration	test0397.co			
1 2 3 4 5 6 7 8 9 9 10 11 12 13 14 15 16 17	0,-1.3754834437 0,-0.3728418073 bp rb31yp/3-21g force test scf=novarace Gaussian Test 3ob 397: Vallnamycin force2 0,1 0,-1.3754834437,-2.5956821846,3.7664927 0,-8.3728418073,-0.5946843,3.8848461 0,-2.381089494,6.53315641668,-0.24838756 0,2.38109894,6.53315641668,-0.24838756 0,2.38109844,3.308408686,-0.26861664 0,2.38109844,3.308408664,0.268616464 0,2.38103874,3.308416864,0.26861643 0,3.927241844,1.9677829583,-2.726165516 0,3.927241844,3.3084745844,3.361661631 0,3.927241844,3.308498694,-3.8386487 0,3.927241844,3.3084758454,3.361661631 0,3.927241845,1.245902434,3.361661531 0,3.927241844,3.308498692,5.383843 0,4.2892751,1.245902434,3.361661531 0,3.927241844,3.364736952,3.38287855 0,3.927241844,3.364736952367,3.38287855 0,3.927241844,3.364736952367,3.38287855 0,3.927241844,3.364736952367,3.38287855 0,3.927241844,3.36485245,3.38287855 0,3.927241844,3.36485245,3.38287855 0,3.927241844,3.364854553,3.38287855 0,3.927241844,3.36485255,3.38287855 0,3.927241844,3.364855257,3.38287855 0,3.927241844,3.3648555257,3.38287855 0,3.927241844,3.364855257,3.38287855 0,3.927241844,3.364855557,3.38287855 0,3.927241844,3.3648555557,3.38287855 0,3.927241844,3.3648555557,3.38287855 0,3.927241844,3.3648555557,3.38287855 0,3.927241844,3.3648555557,3.38287855 0,3.927241844,3.3648555557,3.38287855 0,3.927241844,3.3648555557,3.38287855 0,3.927241844,3.34485555557,3.382878555557 0,3.92724184555557 0,3.927241845555557 0,3.92755555 0,3.9275555 0,3.9275555 0,3.9275555 0,3.927555 0,3	, -2.5956821046, 3.76 , -0.530460483, 3.884 7822 7822 886 44 954 15 52 53 53 53 53 53 53 53 53 53 53 53 53 53	564927822 40401686 ×	test0397.co			
1 2 3 4 5 6 7 8 9 9 10 11 12 13 14 15 16 17 18 19	0,-1.3754834437 0,-0.3728418073 ////////////////////////////////////	, -2.5956821046, 3.76 , -0.530460483, 3.884 	564927822 10401686 × constants	test0397.co			
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	O, -1.3754834437 O, -0.3728418073 b, -0.3728418073 b, -0.3728418073 b, -0.3728418073 b, -0.3728418073 b, -0.372843437, -2.5956821046, 3.7664927 b, -1.3754834437, -2.5956821046, 3.7664927 b, -1.3754834437, -2.5956821046, 3.7664927 b, -1.372418473, -2.5956821046, 3.7664927 b, -1.372418473, -2.5956821046, 3.7664927 b, -2.391890394, 0.5231526187, 1.79968343 c, -2.391890394, 0.5231526187, 1.79968343 c, -2.391890394, 0.5231526187, 1.79968343 c, -2.391890394, 0.5231526187, 1.79968343 c, -2.391890394, -2.3956821046, 0.7864927 c, -2.392741841, 1.9677929589, -2.635814 c, -2.219187407, -1.66738969, -2.635814 c, -2.2586726219, 0.965906551, -3.78843875 c, -2.5586726219, 0.965906551, -3.3887855 c, -0.5281133832, -2.3890727819, 0.2344267	, -2.5956821046, 3.76 , -0.530460483, 3.884 	564927822 10401686 × Constants	test0397.co			

**Gaussian Version Selection** 

#### 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       64     128	8	16 32	
	8			
Select a value between 1 and 64, or 128				
Maximum Execution	72	0	0	
Time	Hours	Minutes	Seconds	
<ul> <li>Use large scratch area</li> <li>Use a slower but larger capacity scratch area.</li> <li>Suitable for large-scale calculations.</li> </ul>				
🚯 Advanced Settir	igs		~	
Advanced Settings (C	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)

l 谷 Advanced Settin	Advanced Settings			
$\Box$ Send email notifications				
Receive email notification and ends	is when the job starts			
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