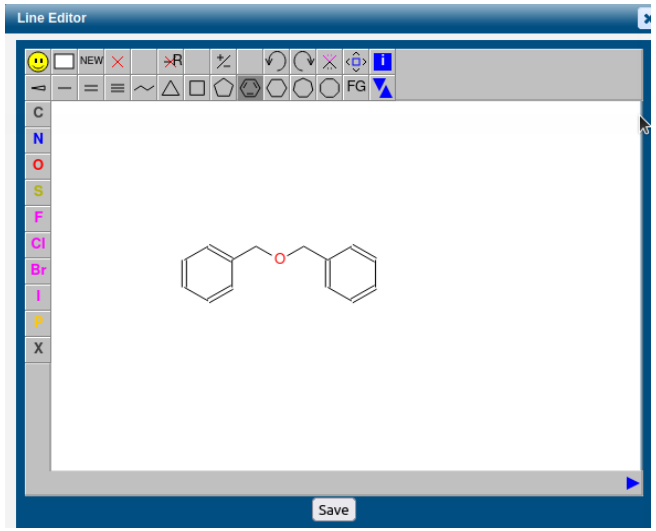
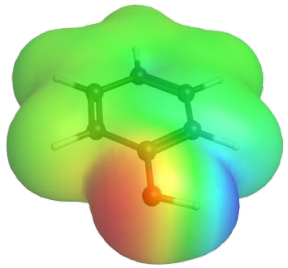
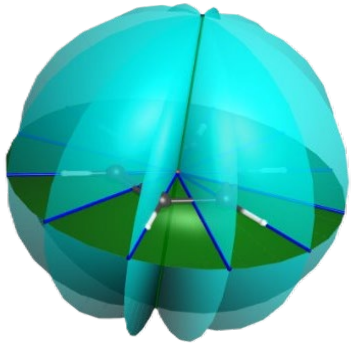
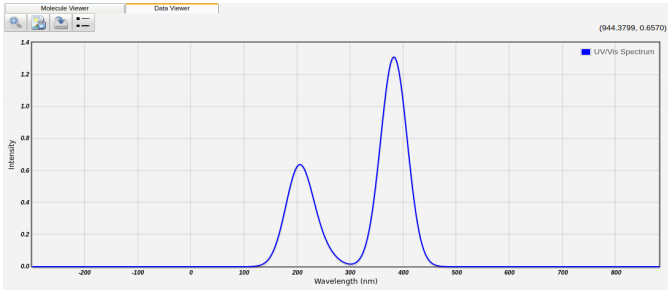




Explore





Build and Submit

Analyze

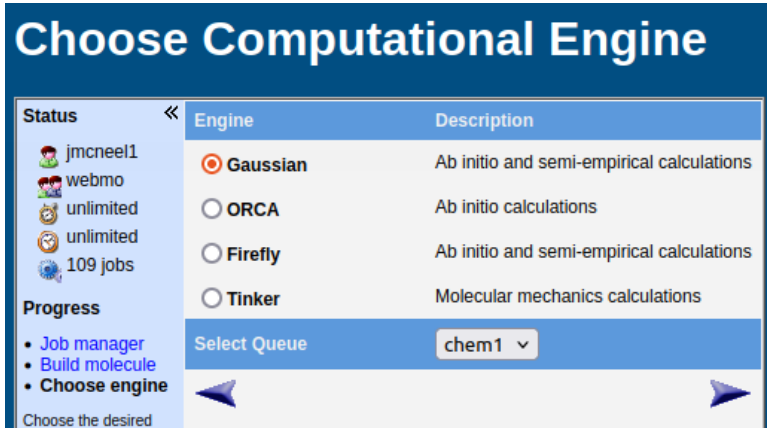
WebMO

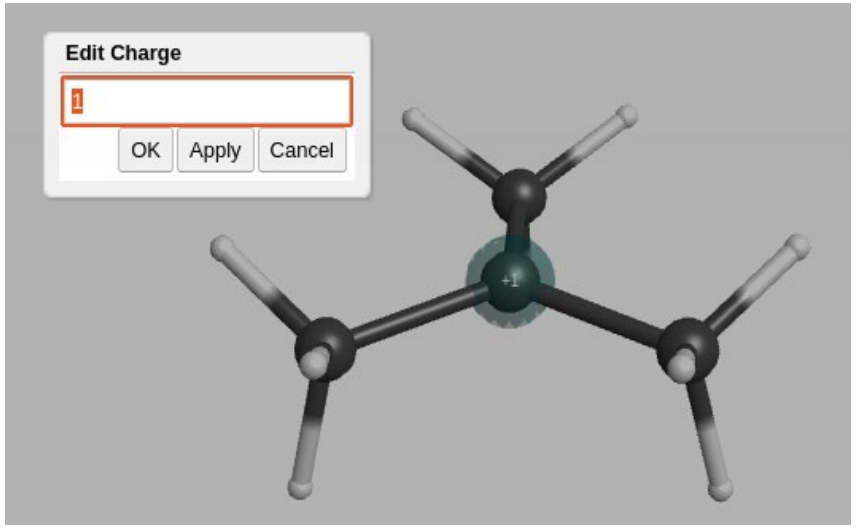
WebMO

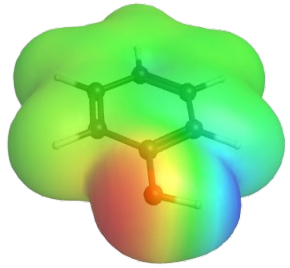
WebMO is a web-based interface interface to powerful computational engines.

Common tasks required to submit jobs to computational engines and analyze results from these engines are automated and simplified.

WebMO also has excellent built-in tools to explore the properties of a molecule before probing the molecule with more advanced computational models.







What are you responsible for?

1. The geometry
2. The charge
3. Is the molecule closed shell or open shell?
4. The basis set for mathematical description of the MOs
5. The computational model (DFT, Hartree-Fock, post-HF, etc...)
6. The calculation (Energy, Geometry Optimization, TD-DFT, etc...)

$$\hat{H} =$$

$$-\sum_{i}^{N_{el}} \frac{1}{2}\nabla_{i}^{2}$$

$$-\sum_{i}^{N_{el}} \sum_{A}^{N_{nuc}} \frac{Z_A}{r_{iA}}$$

$$+\frac{1}{2}\sum_{ij}^{N_{el}} \frac{1}{r_{ij}}$$

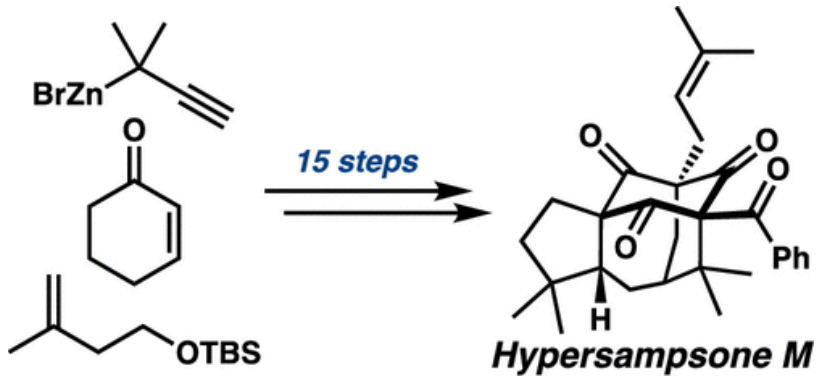
$$+\frac{1}{2}\sum_{AB}^{N_{nuc}} \frac{Z_A Z_B}{r_{AB}}$$

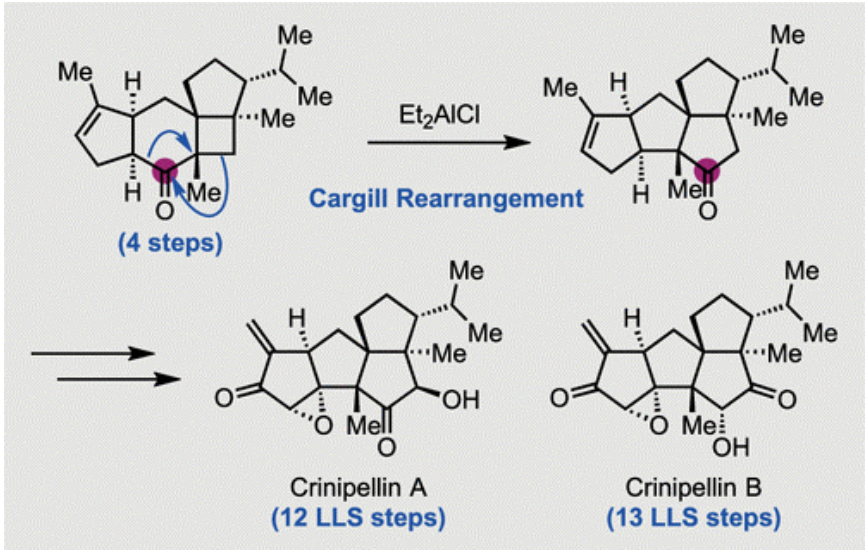
Building and Submitting

1. Use Chemdraw and import the SMILES
2. Lookup by name
3. Building manually with the line editor
4. Building manually with the 3D editor
5. Build using the fragments
6. Import from a file

Building and Submitting

Let’s look at two articles from the “Most Read” listing from JACS (as of late August 2024):





Adrian E. Samkian, Scott C. Virgil, and Brian M. Stoltz
Journal of the American Chemical Society **2024** *146* (28), 18886-18891
DOI: 10.1021/jacs.4c07007

Bo Xu, Ziyao Zhang, Dean J. Tantillo, and Mingji Dai
Journal of the American Chemical Society **2024** *146* (31), 21250-21256
DOI: 10.1021/jacs.4c07900

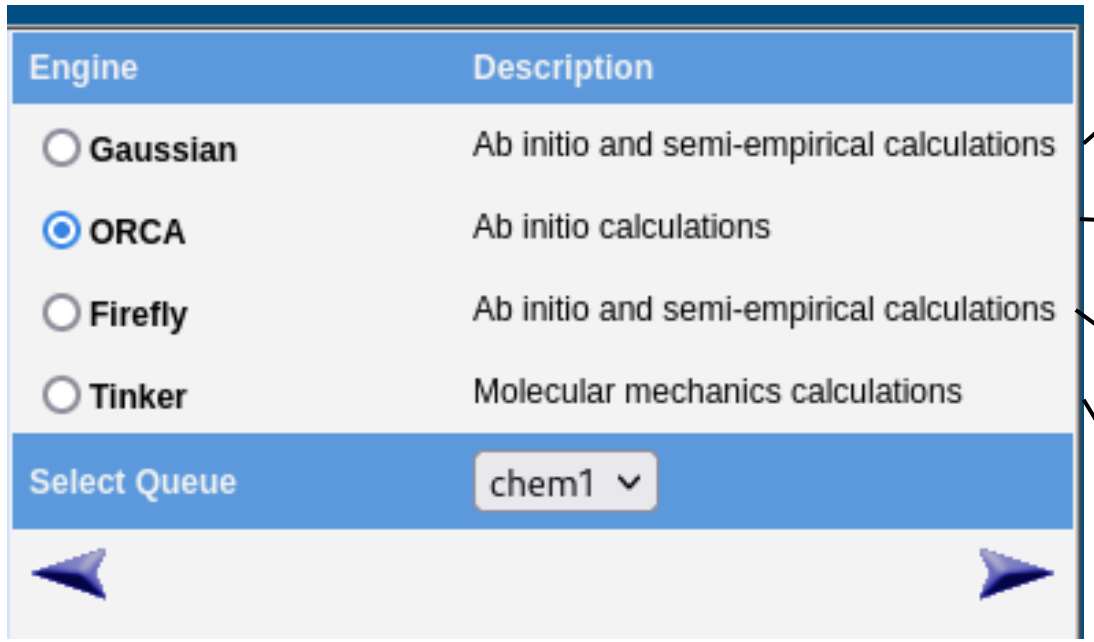
Building and Submitting

The most common mistakes I see people make

1. Don’t forget the protons!!!
2. Errant atoms
3. Forgetting to “clean” the structure
4. Not double-checking the stereochemistry
5. Not properly considering the charge of the molecule

Building and Submitting

Next We Submit, and our first task is to choose an engine



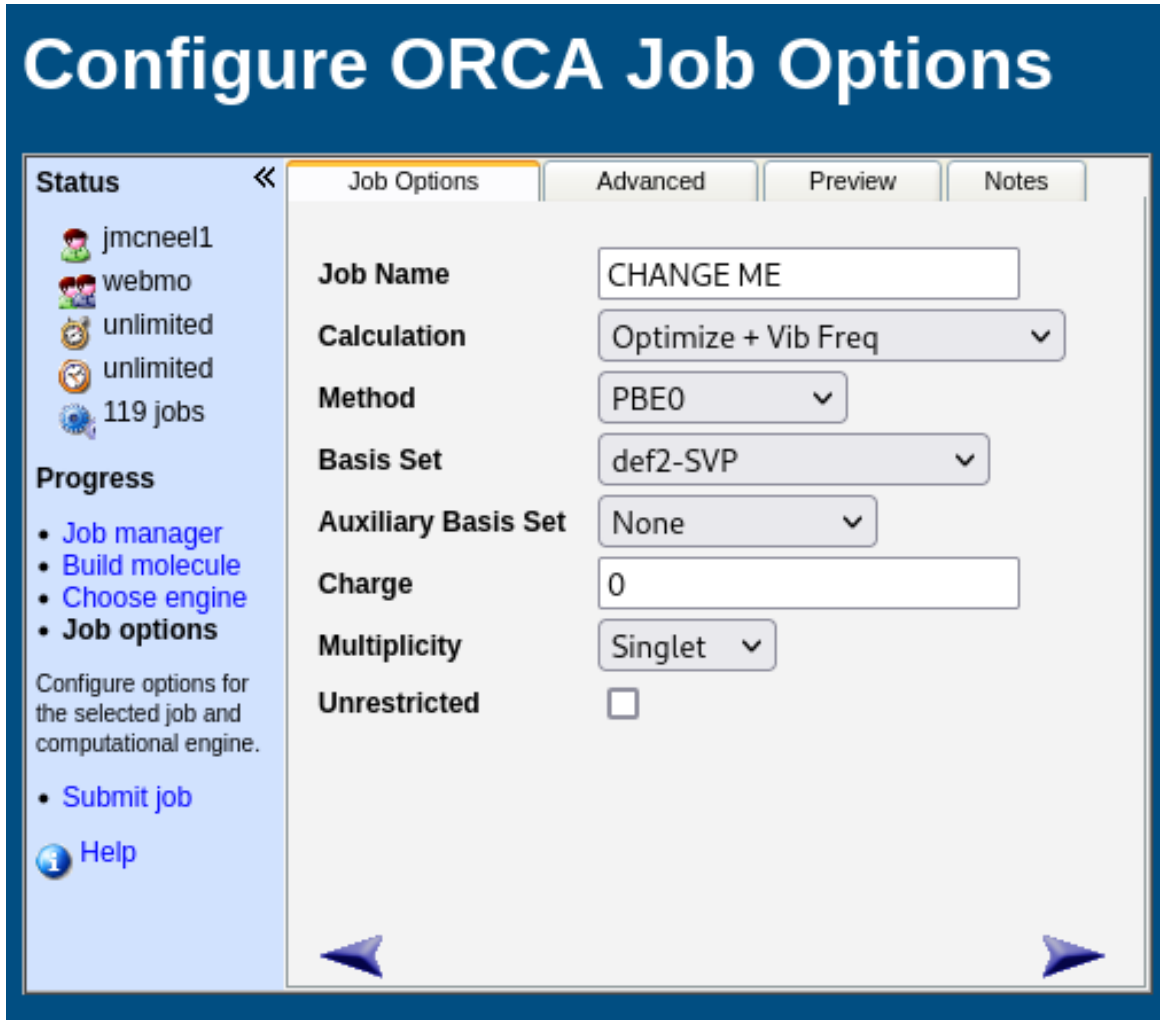
A standard … highly reliable methods. Good choice for DFT, HF energies & optimizations
Two tutorials in Nov/Dec

Offers everything Gaussian offers plus more. A little faster, OPT algorithm a little less reliable…
MANY TUTORIALS TO COME

Less well-known … similar performance to Gaussian with novel high-level technique we won't be covering.

Only force-field energies, only used for conformational analysis…

Building and Submitting

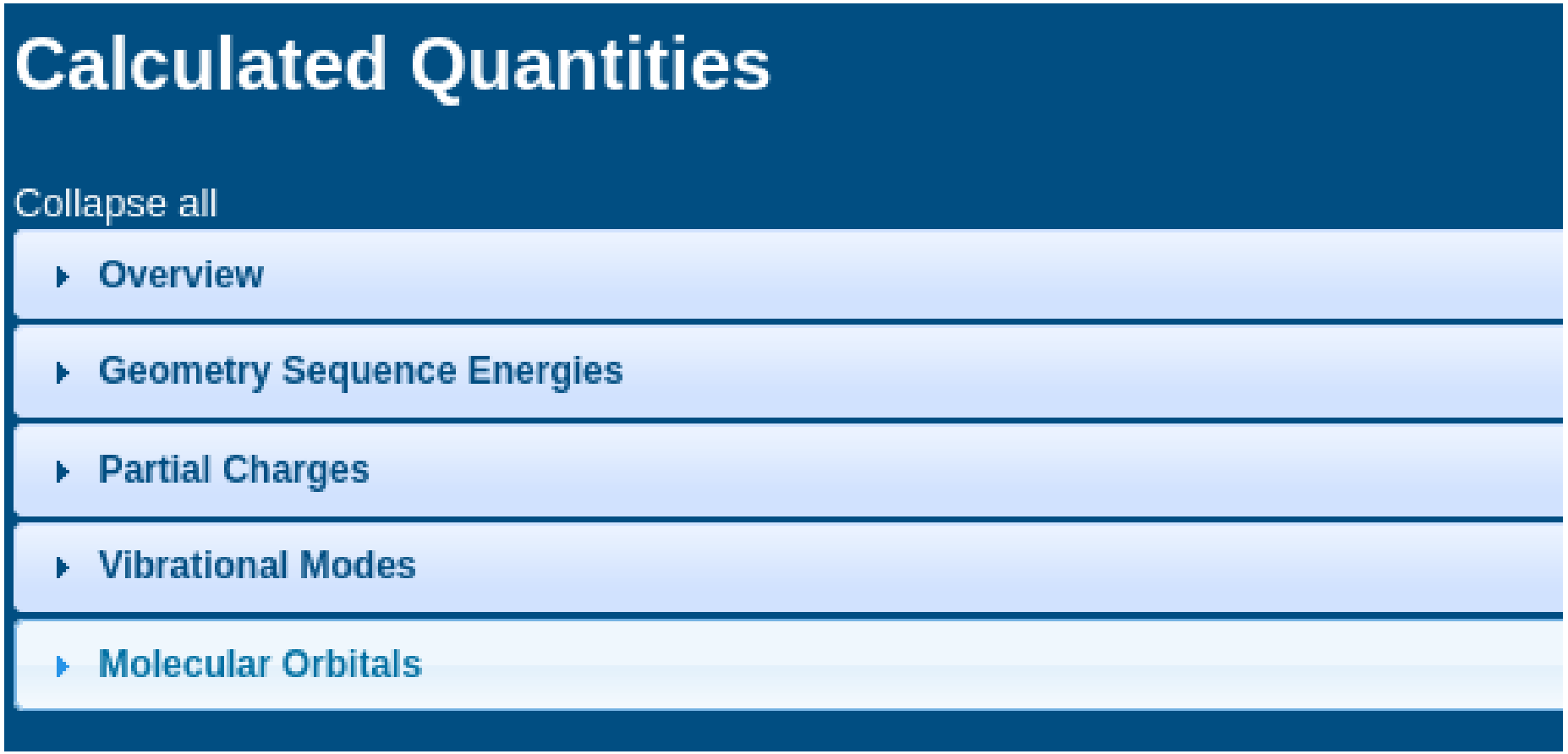


Building and Submitting

Things to remember

1. Don’t forget the charge and multiplicity!!!
2. Don’t forget to set the number of cores in advanced
3. D3BJ is almost always a good idea for optimizations
4. If you want to use a solvent, remember it’s in the advanced section
5. A good Job Name will be helpful a year from now…
6. You have FULL CONTROL with the preview tab if you want to run something more exotic

Analysis – Geometry Optimization + Vib. Freq.



Analysis – Excited States and UV-VIS

Analysis – NMR

Analysis – Natural Bond Orbitals