Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Introduction to IQmol

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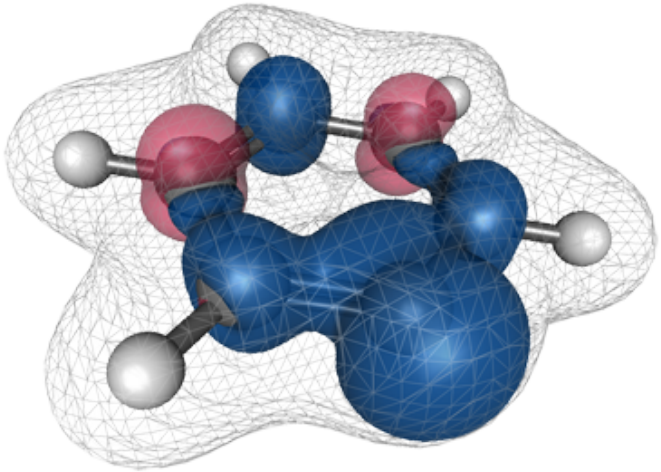
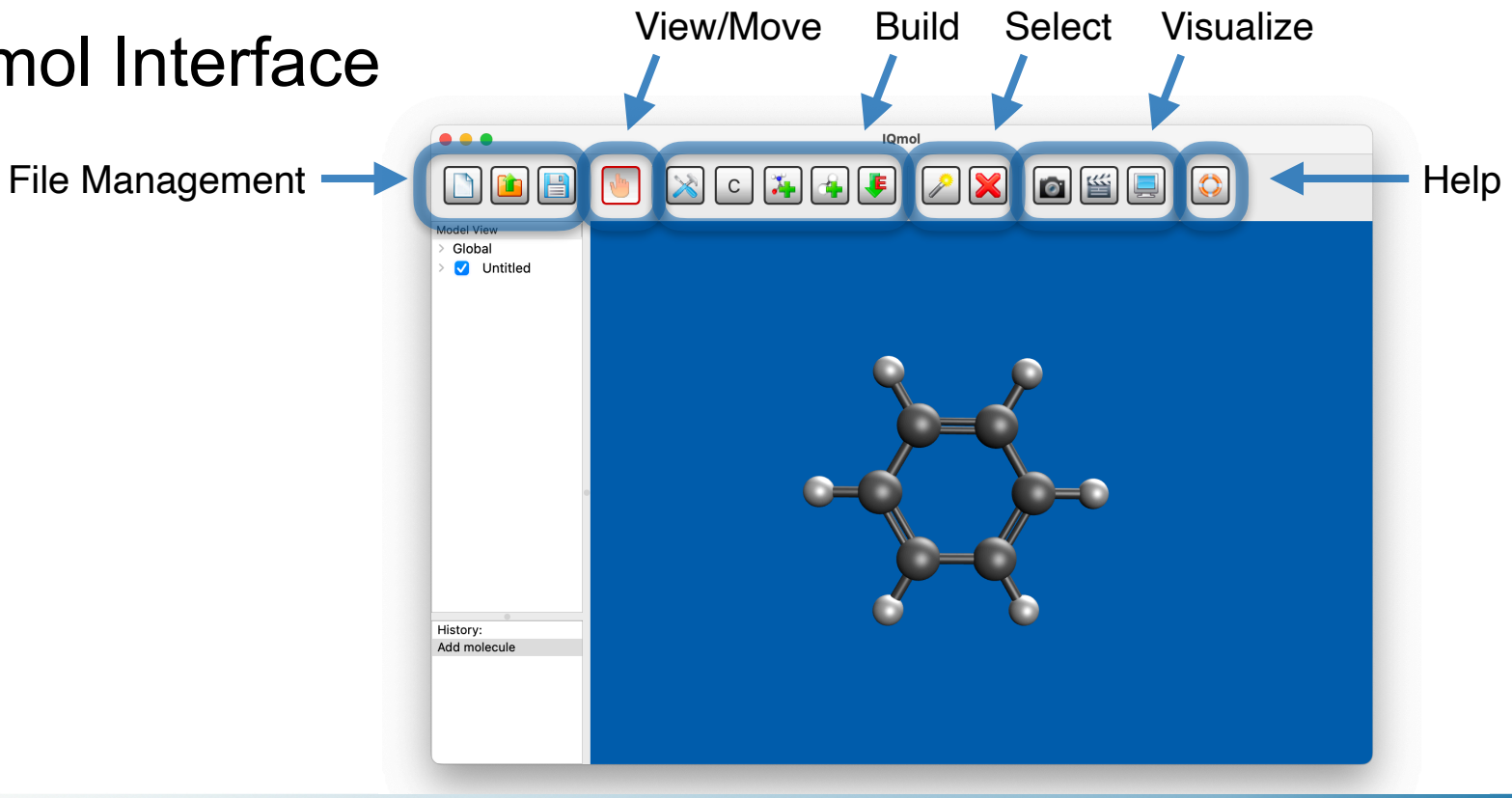
About IQmol

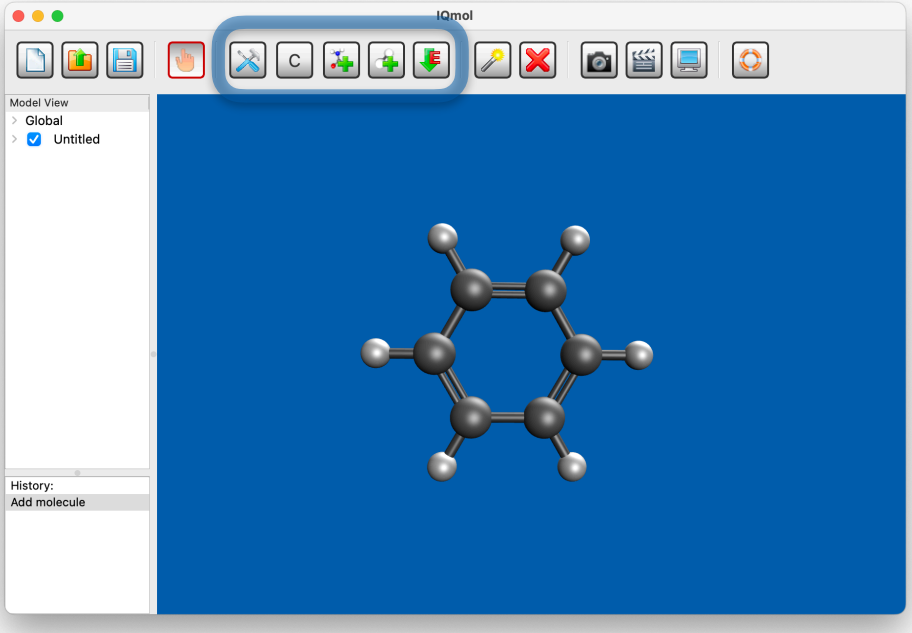
- IQmol is a free, open-source GUI for Q-Chem
- Submit jobs several ways:
  - Submit via IQmol to Q-Chem server (10-min limit)
  - Submit via IQmol to your copy of Q-Chem
  - Construct in IQmol and submit separately



IQmol Interface



Building Molecules



Build Mode

Add Element

Add Fragment

Add Hydrogens

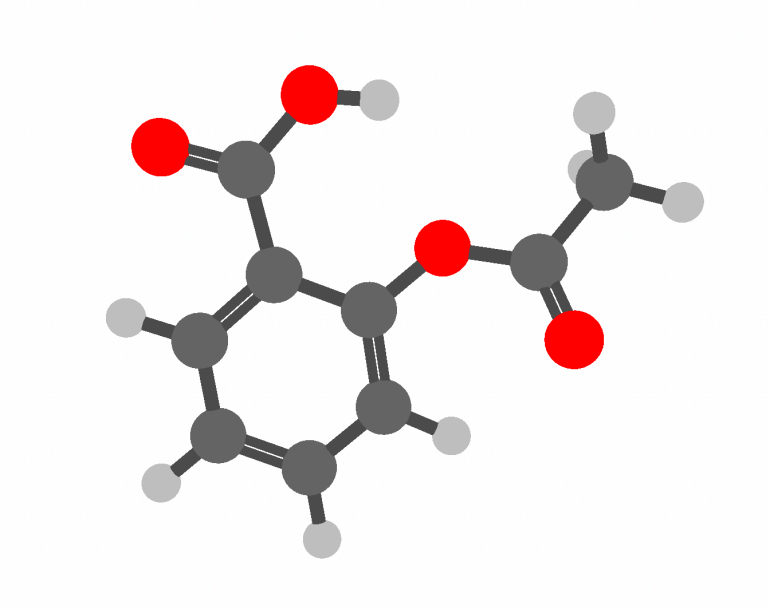
Minimize Energy

Select Tool

Delete Selection

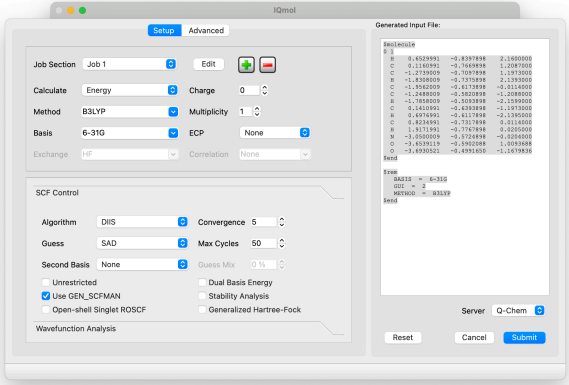
Demo: Building Aspirin

- Start from base structure (anisol)
- Demonstrate:
  - Adding/removing atoms
  - Add hydrogens
  - Build vs. View Mode
  - Constrain angle
  - Minimize energy
  - Measuring angles/bonds

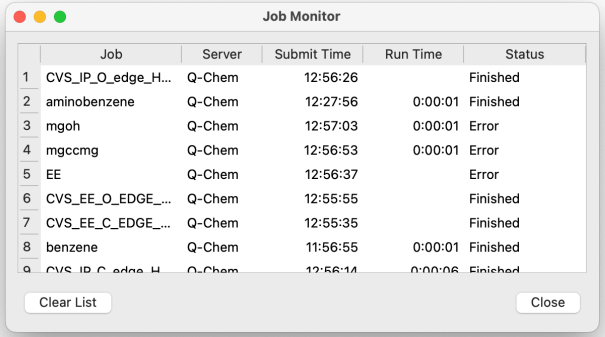


Running Calculations

- Calculation Menu > **Q-Chem Setup**
  - Lets you set up jobs
  - Edit inputs via interface or directly
  - Submit jobs to Q-Chem or local server

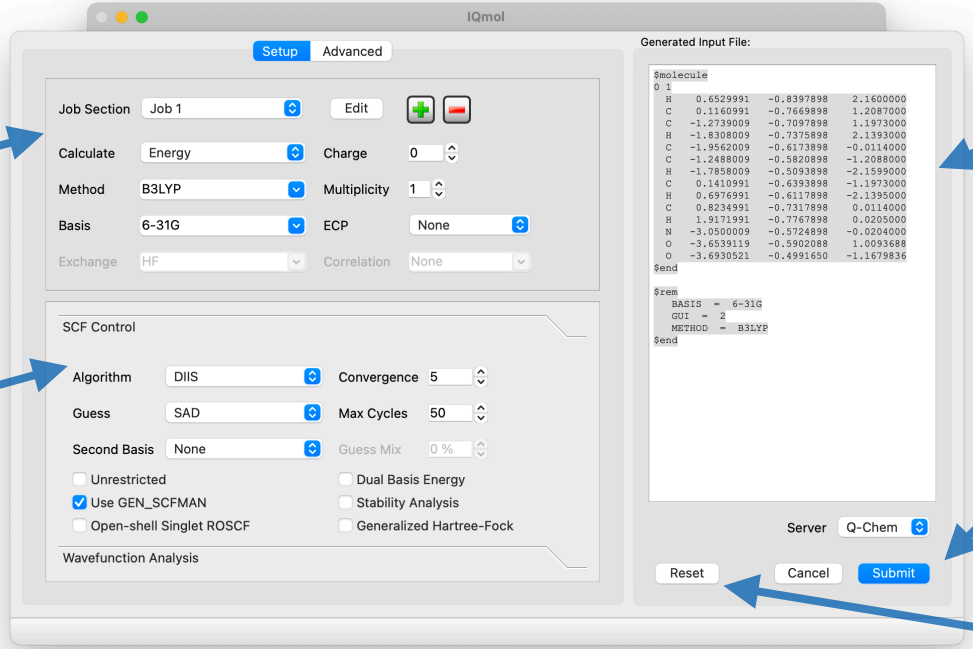


- Calculation Menu > **Job Monitor**
  - Monitor progress of jobs
  - View old/completed jobs



	Job	Server	Submit Time	Run Time	Status
1	CVS_IP_O_edge_H...	Q-Chem	12:56:26		Finished
2	aminobenzene	Q-Chem	12:27:56	0:00:01	Finished
3	mgoh	Q-Chem	12:57:03	0:00:01	Error
4	mgccmg	Q-Chem	12:56:53	0:00:01	Error
5	EE	Q-Chem	12:56:37		Error
6	CVS_EE_O_EDGE_...	Q-Chem	12:55:55		Finished
7	CVS_EE_C_EDGE_...	Q-Chem	12:55:35		Finished
8	benzene	Q-Chem	11:56:55	0:00:01	Finished
9	CVS_IP_C_edge_H...	Q-Chem	12:56:14	0:00:06	Finished

Q-Chem Setup Menu



Job Setup

Details

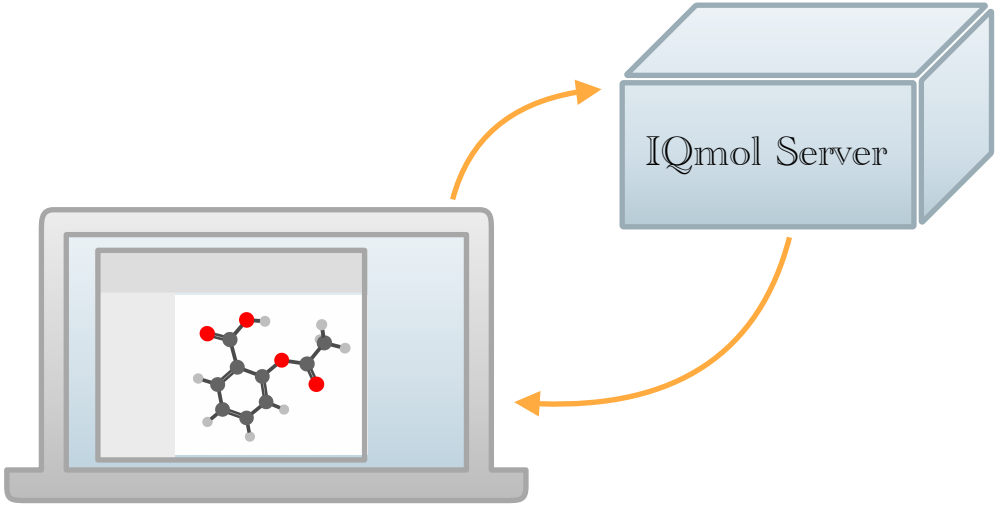
Input

Submit

Reset (use between jobs to clear REMs)

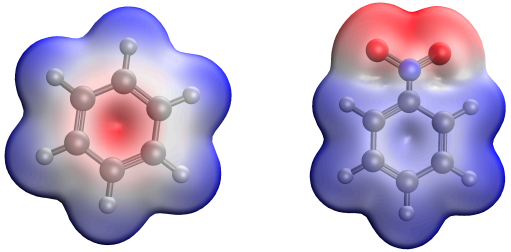
Demo: Submitting Jobs

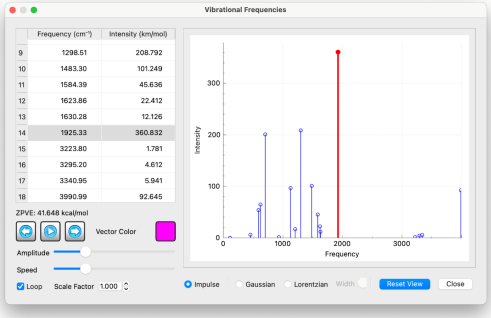
- Demonstrate:
  - Input file setup
  - Submission process
  - Job monitoring
  - Copying results back

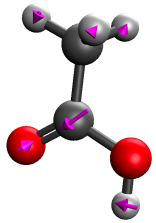


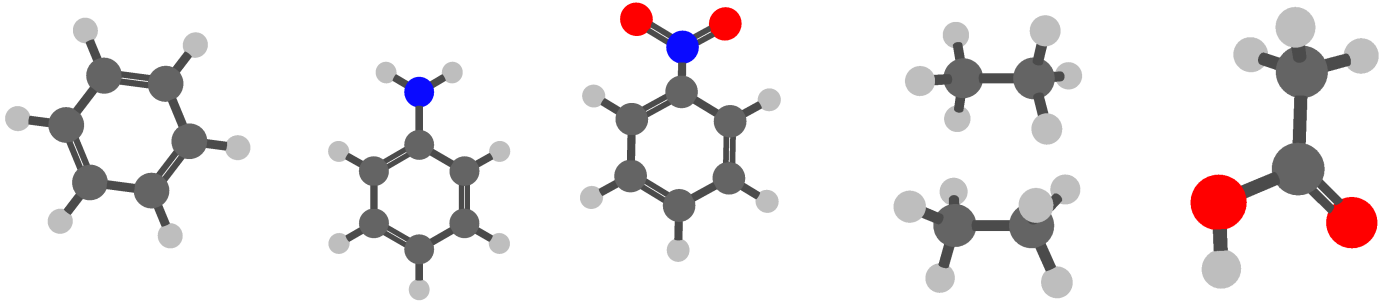
Analyzing Output

- View raw output files under Files > file.out
- Molecular Surfaces
  - Molecular Orbitals (Canonical, Dyson)
  - Total Density, Mulliken (ESP)
- Track geometry optimization steps
- Generate high-resolution POV-Ray files
- Frequencies, spectra, and more!







Exercises

- Lab 1: Basic Building
- Lab 2: Orbital Visualization
- Lab 3: Multiple Jobs & Visualizing Spectra