Introducing the Gaussian Orion Module

Varsha Jain

Application Scientist II

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QM Calculations on the Orion® Platform

Suites of **scientific** methods as turnkey solutions

- *Small Molecule* Discovery Suite
- *Antibody* Discovery Suite
- *Formulations* Suite
- Gaussian — *Gaussian Orion Module (3rd Party)*
- *To Be Announced* Suite

Core technology platform

- Orion®

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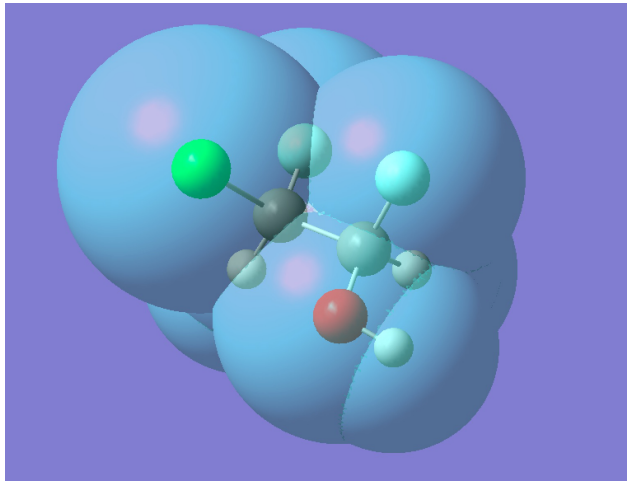
Many Thanks to….

Caitlin Bannan

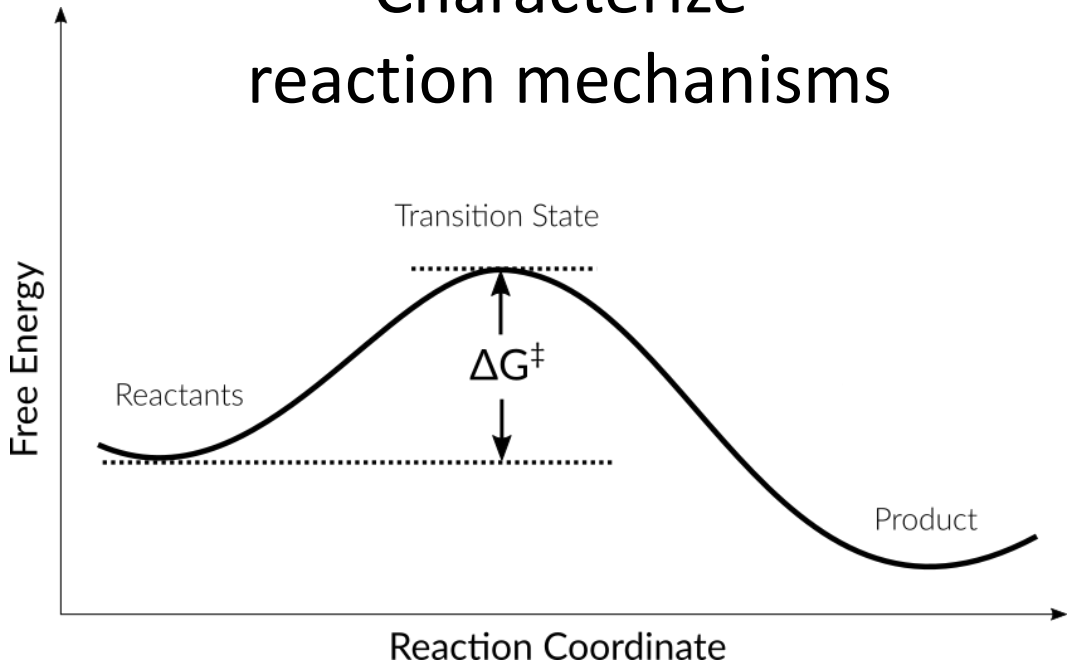
Fred Livingston

Gaussian Extends QM Capabilities

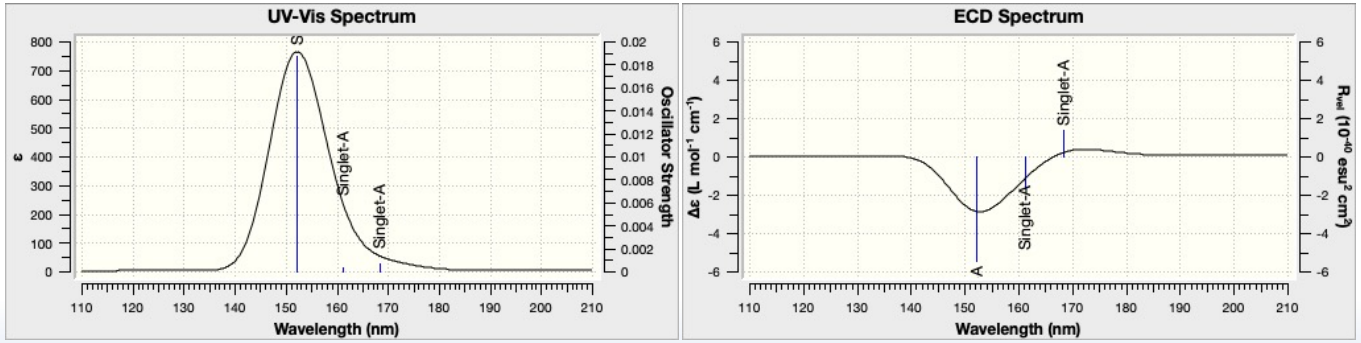
Solvent models with gradients



Characterize reaction mechanisms



Spectra Predictions



Molecule and Spectra created in GaussView, rxn coordinate: https://www.scm.com/doc/Tutorials/StructureAndReactivity/ZN-PES-Scan_TST.html

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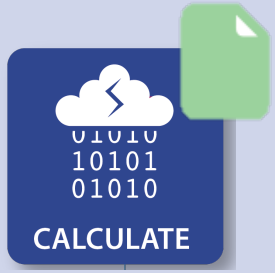
How can you use Gaussian on Orion?

Method	Pros	Cons
Run Gaussian input files with Orion as a computational engine	• Unlimited flexibility 	• Gaussian expertise required • Analysis off Orion

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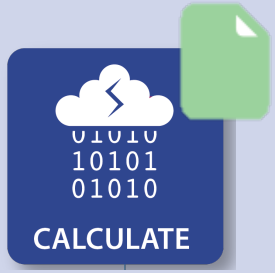
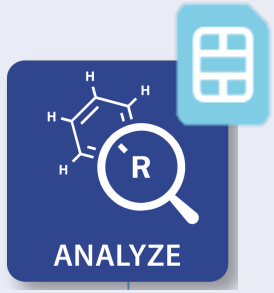
Run Gaussian input files with Orion as a computational engine	• Unlimited flexibility 	• Gaussian expertise required • Analysis off Orion
QM properties calculated on Orion datasets	• No Gaussian expertise 	• Limited functionality single point energy and geometry optimization only

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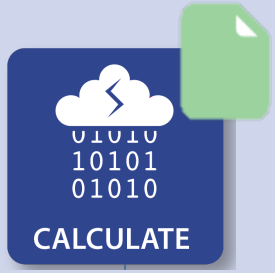
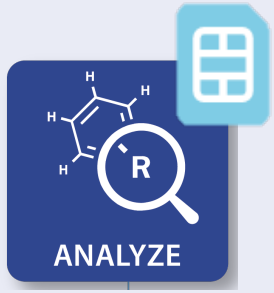
Run Gaussian input files with Orion as a computational engine	• Unlimited flexibility 	• Gaussian expertise required • Analysis off Orion
QM properties calculated on Orion datasets	• No Gaussian expertise 	• Limited functionality single point energy and geometry optimization only

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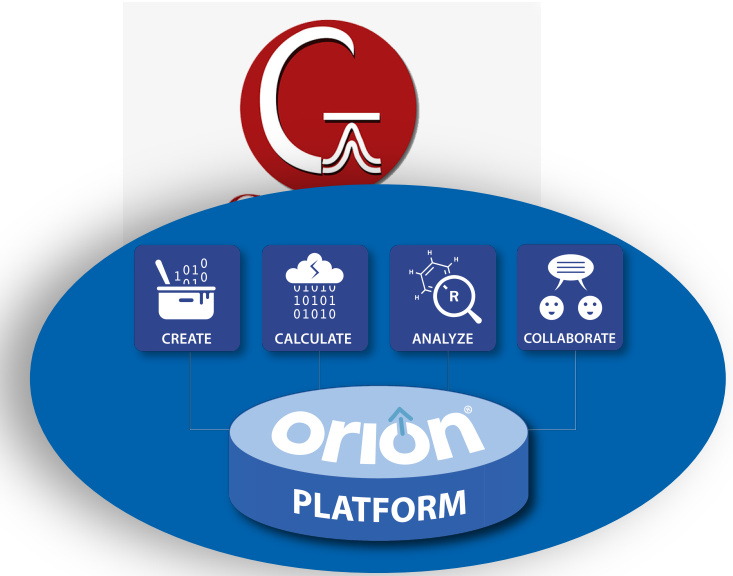
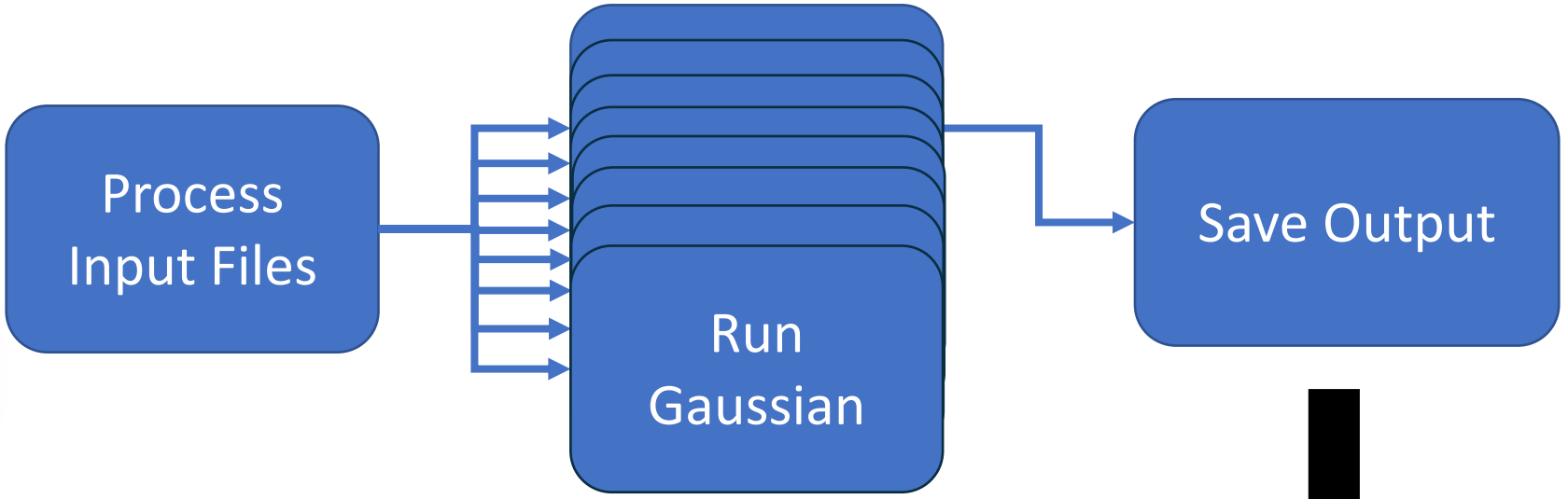
Run Gaussian on Orion





Non-spot, serial Cubes

Input

- Gaussian input file (.com/.gjf)
- Many saved in a Tar or Zip file

Output

- Tar file saving output
- Sub-directory/calculation

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Example Input and Output Format

Input Files

- Input1.com
- Many_inputs.tar
  - Dir1
    - Input2.com
    - Check.chk
  - Input3.gjf

Output Tar

- Input1
  - Input1.com
  - Input1.log
- Dir1
  - Input2.com
  - Check.chk
  - Input2.log
- Input3
  - Input3.gjf
  - Input3.log
  - Freq.chk
  - Freq.cube

Checking Gaussian Input Files

Fails before running Gaussian

- Hardware requirements
  - No GPU support

benzoic_acid1.com — Editec

```
%GPUCPU=0,1,2,3,4,5=0,1,16,17,18,19
%Chk=benzoicacid1.chk
# B3LYP/6-31G(d) Opt

 Title

0 1
C          0.82690         1.11080         0.16720
C          0.53230         0.64730        -1.11500
C         -0.29460        -0.46350        -1.28220
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C         -0.53230        -0.64730         1.11500
C          0.29460         0.46350         1.28220
C         -1.68900        -2.26880        -0.34130
O         -2.01470        -2.76280        -1.42590
O         -2.12090        -2.77930         0.84440
H          1.47130         1.97520         0.29720
H          0.94670         1.15110        -1.98370
H         -0.51670        -0.81580        -2.28620
H         -0.94180        -1.14390         1.99100
H          0.52440         0.82370         2.28070
H         -2.70320        -3.56150         0.73790
```

Details of Failed calculations:
This input file requests GPU calculation. We do not support GPU Gaussian calculations at this time. Please update your input file and try again.:
* benzoic_acid_gpu

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Checking Gaussian Input Files

Fails before running Gaussian

- Hardware requirements
  - No GPU support
  - More CPUs/memory/disk than asked for in the Orion Floe

benzoic_acid_others.com — Edited

```
%Mem=20GB
%maxdisk=30GB
%CPU=0-10
%Chk=benzoicacid1.chk
# B3LYP/6-31G(d) Opt

 Title

0 1
C          0.82690        1.11080        0.16720
C          0.53230        0.64730       -1.11500
C         -0.29460       -0.46350       -1.28220
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H          0.52440        0.82370        2.28070
H         -2.70320       -3.56150        0.73790
```

Details of Failed calculations:
This input file had the memory line Insufficient resources requested on Orion, which failed with the message %Mem=20GB The Orion hardware requirement was set to 14400.0MB. Update the input file or the specified hardware requirements and try again.:
* benzoic_acid_others

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Checking Gaussian Input Files

```
%Chk=benzoicacid1.chk
# B3LYP/6-31G(d) Opt

 Title

0 1
C           0.82690         1.11080         0.16720
C           0.53230         0.64730        -1.11500
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~
~
~
~
~
~
~
~
~
~
~
```

Edits file and prints a warning

- File formatting
  - Add missing bottom blank line

Checking Gaussian Input Files

benzoic_path.com — Edited

```
%Chk=scratch/vjain/gaussian/benzoic.chk
# B3LYP/6-31G(d) Opt

 Title

0 1
C          0.82690        1.11080        0.16720
C          0.53230        0.64730       -1.11500
C         -0.29460       -0.46350       -1.28220
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```

Edits file and prints a warning

- File formatting
  - Add missing bottom blank line
- Output file paths
  - All output files must be written to running directory for now

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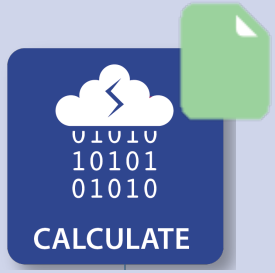
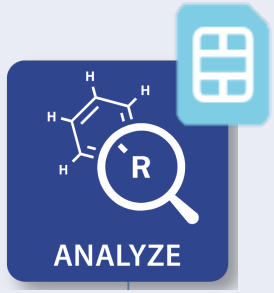
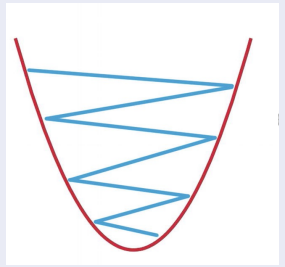
Run Gaussian input files with Orion as a computational engine	• Unlimited flexibility 	• Gaussian expertise required • Analysis off Orion
★ QM properties calculated on Orion datasets	• No Gaussian expertise 	• Limited functionality  

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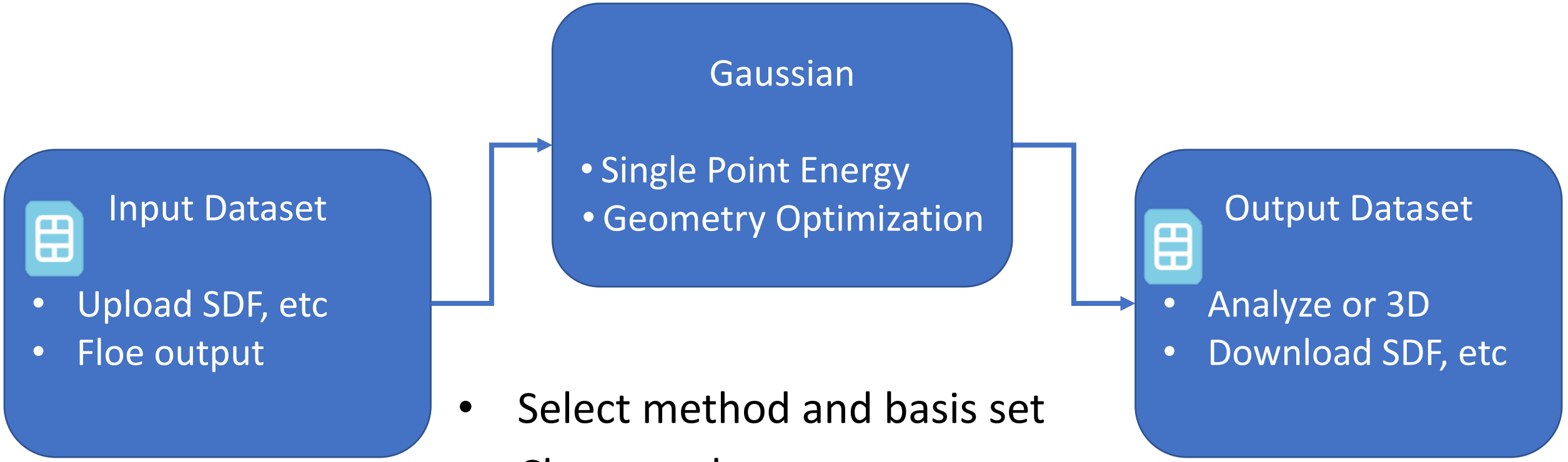
Integrate Gaussian Calculations with Datasets



- Select method and basis set
- Choose solvent
- Exposed hardware requirements

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Choices for Method, Basis Set, and Solvent

Method Options

- ✓ HF
- B3LYP
- B2PLYP
- M06
- M062X
- MN15
- CAM-B3LYP
- WB97X
- wB97XD
- LC-wHPBE
- PBE1PBE
- MP2

Basis Set Options

- 3-21G
- ✓ 6-31G
- 6-31G*
- 6-31+G*
- 6-31G**
- 6-31+G**
- 6-311G**
- 6-311+G**
- 6-311G(2d,2p)
- def2SVP
- def2TZVP
- def2TZVPP
- aug-cc-pvdz
- aug-cc-pvtz

Solvent Options

- ✓ Gas Phase
- Water (IEF-PCM model)

Check for Hardware Metrics

Future release will have….

- Better Gaussian failure handling

- Integration with OpenEye Toolkits for
  - Torsion scans
  - Conformer ensembles
  - Tautomer Analysis

- Better integration with Gaussian output

Tutorials

- How to run each Floe:
  - Run Gaussian input files – Success and Failures
  - Single point energy on benzoic acid
  - Geometry optimization in gas phase and water

- FAQ Section
  - How to check metrics?
  - Why are there so many serial cubes?
  - What method and basis set should I use?
  - … etc

https://docs.eyesopen.com/floe/gaussian-module/index.html

Thank You

For more information, please contact:

sales@eyesopen.com | **info@eyesopen.com**

www.openeye.inc

+1-505-473-7385

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