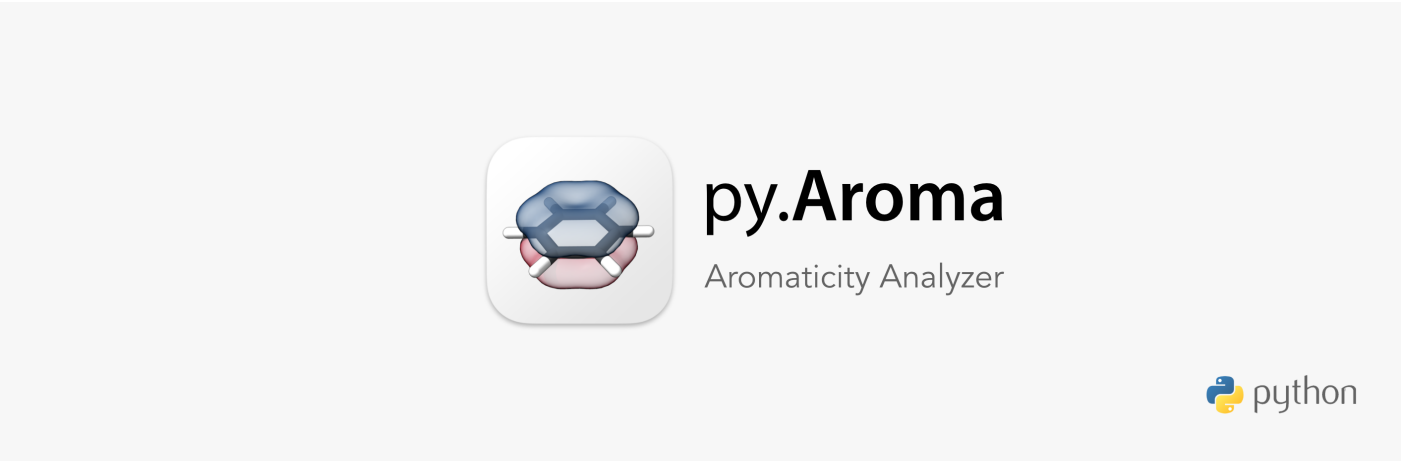
py.**Aroma** 2



Latest version: **2.1.0**, updated at 2023-01-14

1. Statement of need

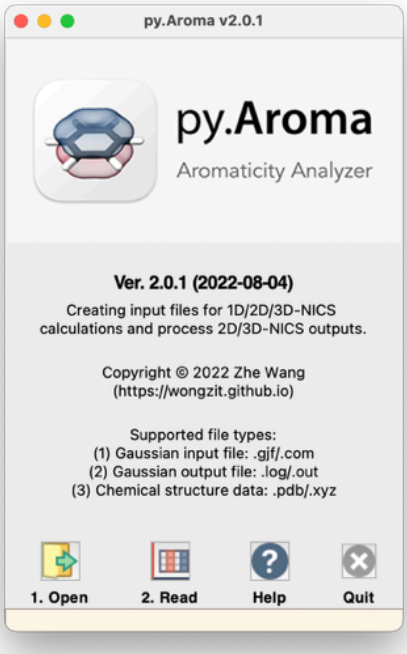
py.**Aroma** is a Python program for aromaticity analyses. Users can easily create input files for NICS, 2D-NICS and 3D-NICS calculations and process output files of 2D-NICS and 3D-NICS calculations.

2. Usage

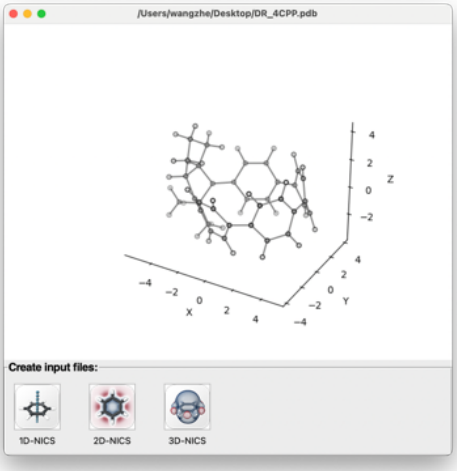
2.1 General

py.**Aroma** can read *Gaussian* type input files (*.gjf* and *.com*), *.pdb* files and *.xyz* files for creating NICS input files. *Gaussian* type output files (*.log* and *.out*) could be used for processing 2D-NICS and 3D-NICS outputs by py.**Aroma**.

The start window of py.**Aroma** is like following.

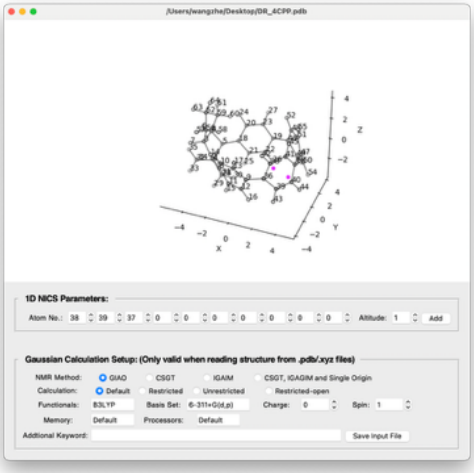


User need to start from the  **1. Open** icon to read a file, and click  **2. Read** to display the structure.



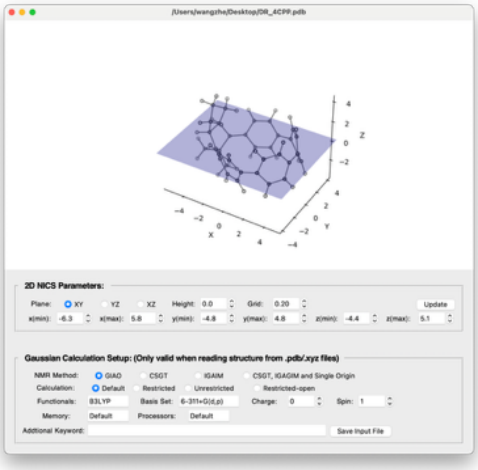
2.2 Creating NICS Input Files

Users can go to input file setting window by clicking the **1D-NICS**, **2D-NICS** and **3D-NICS** button. For **1D-NICS**, users need to specify the atom numbers. The ghost atom for NICS(0) would be added at the center of the specified atoms. By inputting the altitude, two ghost atoms would be added below and over the plane. Users can check the preview of ghost atom by clicking *update* button.

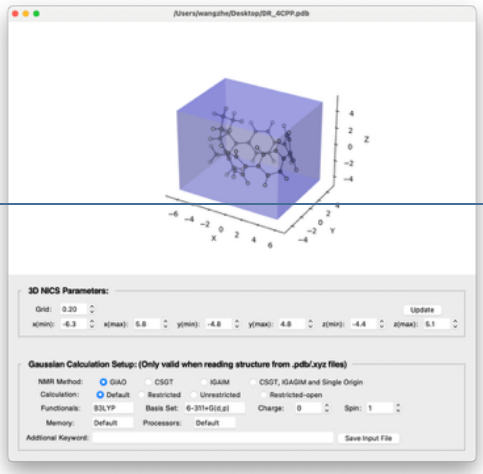


For the geometries inputted by *.pdb* and *.xyz* files, users can set the *Gaussian* calculation keywords in the **Gaussian Calculation Setup** part. Click *Save Input File* will save the input files to the same dictionary of geometries inputs. Reading geometries from *.gjf* or *.com* files, the **Gaussian Calculation Setup** part is useless, the new generated input file will read keywords from the original input files.

For 2D-NICS, users need to specify the plane (XY, XZ or YZ), range, grid space and altitude. Users can also preview the position of ghost atoms by clicking the *update* button.



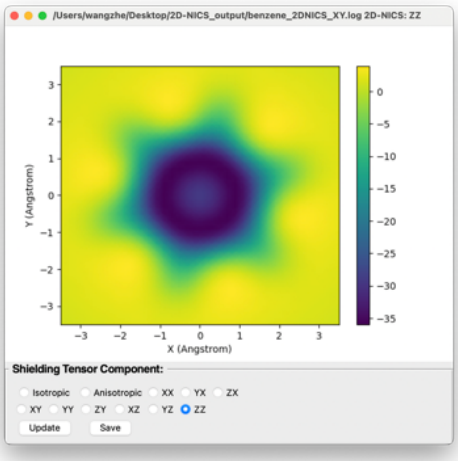
For 3D-NICS, users need to specify the range and grid spacee. Users can preview the cube of ghost atoms by clicking the *update* button.



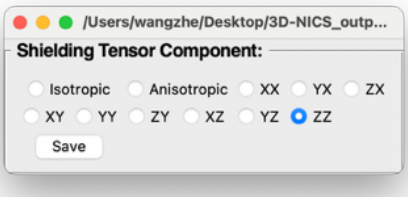
2.3 Processing NICS Output

py.**Aroma** can process 2D-NICS and 3D-NICS output files which calculated from the input files generated by py.**Aroma**. By open a *.log* or *.out* file to py.**Aroma**, the program will determine the type of 2D- or 3D-NICS output.

For 2D-NICS, py.**Aroma** would extract the sheilding tensors from output file, and plot a heat map using built-in module. Users can choose every component of their interests to plot the heat map. By clicking *Save* button, a *.png* file and a *.csv* file contain shelding tensors would be saved.



Similar to 2D-NICS, 3D-NICS output could also be processed by py.**Aroma**. User can also choose the component and save the sheilding tensors to a *.cub* file. The *.cub* file could be visuallized by *GaussView*, *VMD*, *ChimeraX*, etc.


/Users/wangzhe/Desktop/3D-NICS_outp...
Shielding Tensor Component:
Isotropic
Anisotropic
XX
YX
ZX
XY
YY
ZY
XZ
YZ
ZZ
Save