NBOScan 1.0

Application manual

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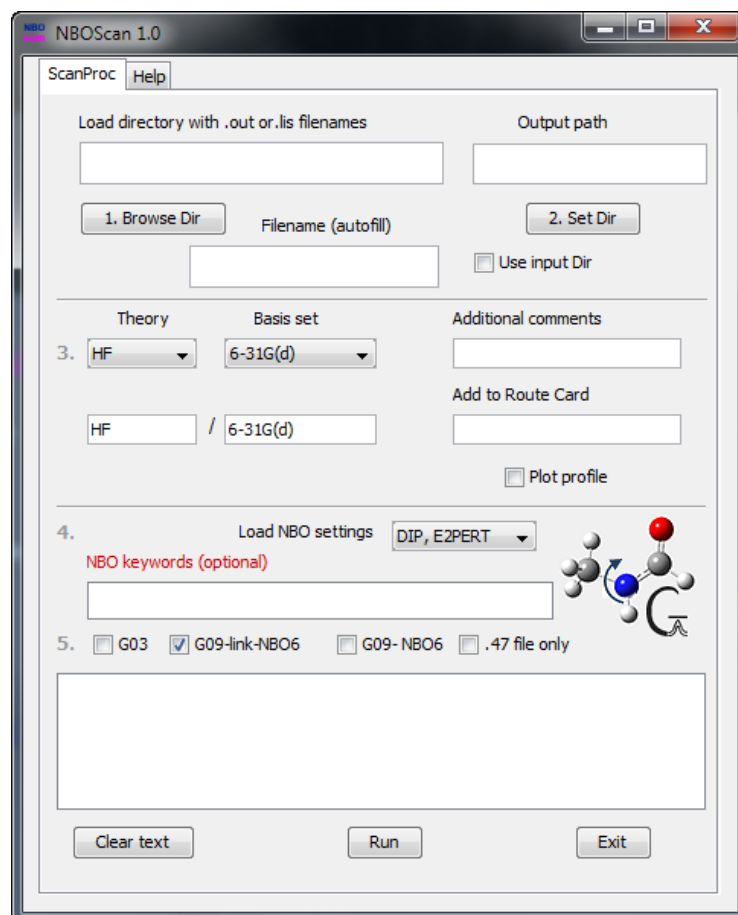
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1.1 What is NBOScan?

NBOScan is java-based application that processes Gaussian output files containing results of the Potential Energy Scan (PES) jobs. NboScan extracts essential parts of the PES output file and creates formatted Gaussian input files (.gjf) to perform a single point NBO analysis. The number of files corresponds to the number of incremental steps in the coordinate scan. Newly created .gjf files include NBO keywords and instructions to perform NBO analysis at each geometry on the PES.

NboScan:

  I.   Reads Gaussian output files containing geometries and energies of the PES scan (output of coordinate driving).
 II.   Generates multiple Gaussian input files (.gjf) containing custom route card, comments, geometries, and NBO keylists with the corresponding keywords.
III.   Generates a plot view of energy profile along the scanned coordinate.
IV.   Creates Gaussian batch list file (.bcf) for processing multiple input (.gjf) files.

NBOScan assumes user's familiarity with NBO programs developed by Frank Weinhold at the University of Wisconsin.

For details on NBO programs, visit NBO6 Website at http://nbo6.chem.wisc.edu

1.2 Recommended Reading

In addition to the NBO6 website link, following resources are invaluable for a better understanding of chemical phenomena predicted by NBO analysis.

- NBO6 manual

- F. Weinhold, "Natural bond orbital analysis: A critical overview of relationships to alternative bonding perspectives," J. Comput. Chem. (2012).

- F. Weinhold and C. R. Landis, Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective (Cambridge U. Press, 2004), 760pp.

- F. Weinhold and C. R. Landis, Discovering Chemistry with Natural Bond Orbitals (Wiley-VCH, 2012), 319pp.

1.3 Why NBOScan?

NBO analysis of orbital interactions is a powerful approach to understanding molecular properties. Subtle interactions can be often revealed by studying the NBO-derived properties at the potential energy surface (PES). By plotting the potential energy changes along the defined molecular coordinate (atom distance, angle, dihedral), one can get a better appreciation of different components of the total energy. The main motivation behind the NBOScan was to simplify analysis of the PES results by parsing the output files into a series of new input files formatted for NBO analysis.

1.4 Requirements

1.4.1 Java 7: NBOScan application is written in Java using JDK1.7 (Java SE 7). Make sure that you have the latest JRE (at least Java7) installed on your computer. You can download the java installer jxpiinstall.exe form here or the latest platform-specific Java from here.

NBOScan was developed and tested under Windows system (Win7). While it should also run under Linux (with Java installed) or Mac OS, there may be issues with file opening and saving due to differences between the systems. If an error message appears upon the launch of NBOScan, first and the most straightforward remedy is to (re)install the latest version of Java.

1.4.2 ESS/NBO Program: to fully utilize all features of NBOScan, Gaussian09 (G09W) or PC-GAMESS/Firefly is recommended for direct interaction with NBO routines. Windows version of G09 is based on the older nbo3.1 code. Since the revision D.01, G09W can now link with

standalone NBO6 binaries via gaunbo6.bat batch script included in the NBO6 package (available from NBO6 website).

PC-GAMESS/Firefly (FF) is freely available *ab initio* and DFT computational chemistry program developed and maintained by Dr. Alex A. Granovsky at Lomonosov Moscow State University (MSU). It can be downloaded from here. To enable NBO analysis in FF, you need to purchase NBO ID and password from NBO6 website.

While ESS, NBO6, and Firefly binaries can be installed at any partition/directory on your system, recommended directories are:

c:\G09W

c:\nbo6w

c:\Firefly

1.4.3 NBOScan Download: download zip file containing all required files and manual from www.marcelpatek.com/nbo/nbo.html See section 1.5 for installation instructions.

1.5 Installation

NBOScan is a self-contained application. It can be run from any file folder on the PC hard drive or optionally from a USB drive. NboScan.zip archive contains the following files:

- NboScan.jar [main java application]
- lib folder containing jfreechart-1.0.17.jar and jcommon-1.0.21.jar libraries
- NboScan_man.pdf [manual for this application]

INSTALL
1. Unzip downloaded NboScan.zip file and move its content into any directory on your system. Recommended place is c:\nbo\NboScan
2. Create shortcut of NBOScan to your Desktop (right-mouse click the file -> Send to -> Desktop (create shortcut)
3. Double-click the shortcut icon to run the application

4. To install nbo6 binaries and supporting files, follow instructions in the NBO6 package [optional]*

* Installation of NBO6w package from [TCI/NBO Software](#) is optional.

2.0 Overview and Usage

Outline of a typical computational workflow for NBO analysis of PES geometries is outlined below (**Figure 1**).
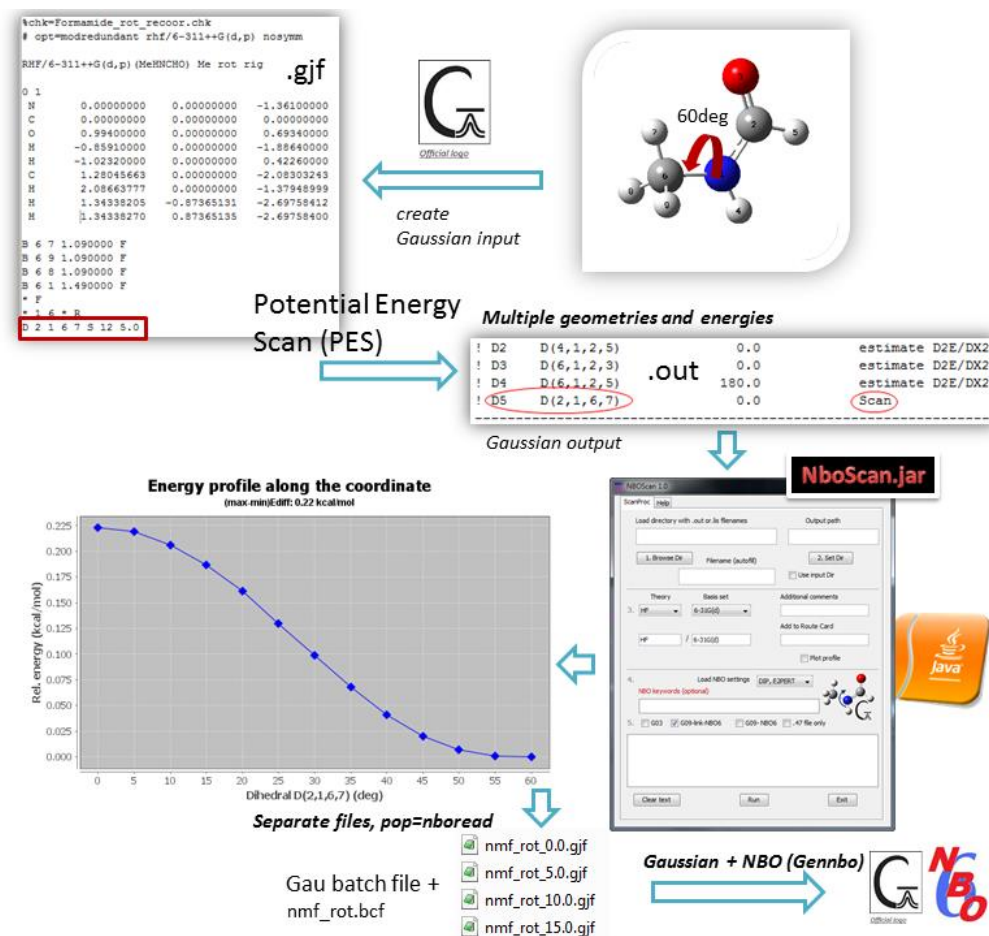
Figure 1

To avoid potential troubles with a poorly constructed Z-matrix, NboScan app can only read output files generated by the relaxed PES scan initiated with the keyword **Opt=ModRedundant**.

In such case, the keyword requests that a geometry optimization (Opt) be performed in redundant internal coordinate that may include scan and constraint information. The latter option requires a separate input section to activate, freeze, and scan PES. Initial geometry can be supplied as Cartesian coordinates or as Z-matrix (top left snapshot). Results are recorded in the job output file (Gaussian output). Each PES output file contains table of "Initial Parameters", which indicate the name and the value of <u>Scanned</u> and <u>Frozen</u> coordinates. Atom coordinates together with the corresponding energy at each coordinate increment are all part of the output file. By running the NboScan application, plot of the energy values along the scanned coordinate is created along with multiple files formatted for a single point calculation of NBO properties (bottom of the snapshot).

2.1 Main window of the graphical user interface

NBOScan graphical user interface consists of three main areas (**Figure 2**):

1) File input (top, 1. and 2.)
2) Options (middle, 3., 4. and 5.)
3) Output (bottom)

To clear text from **sections 3-5**, press button "Clear text". Clicking the "Run" button starts processing of the PES file.
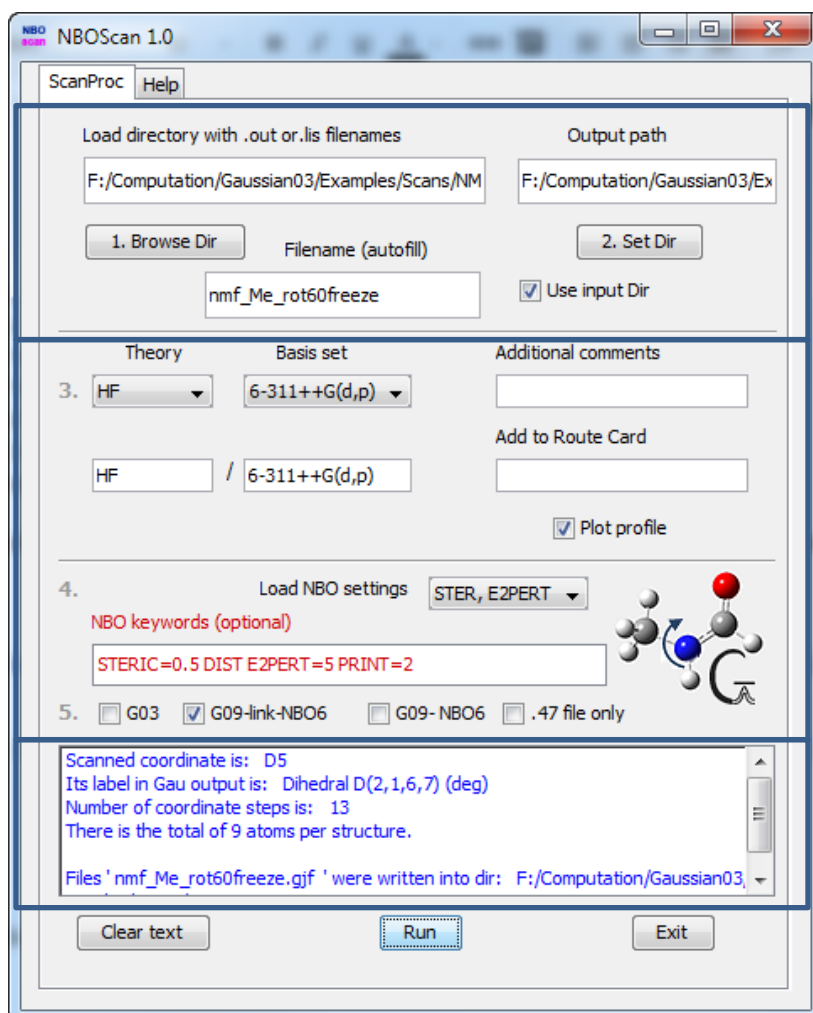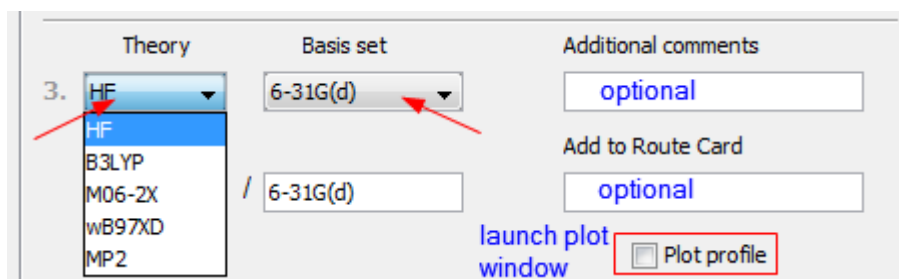

Figure 2

Start by clicking on button **1. Browse Dir** to locate the Gaussian PES output file. Set the output directory for the Gaussian input files (.gjf) created by the run. Use the **2. Set Dir** button. Alternatively, check the **Use input Dir** box to direct output into the same directory (**Figure 3**).
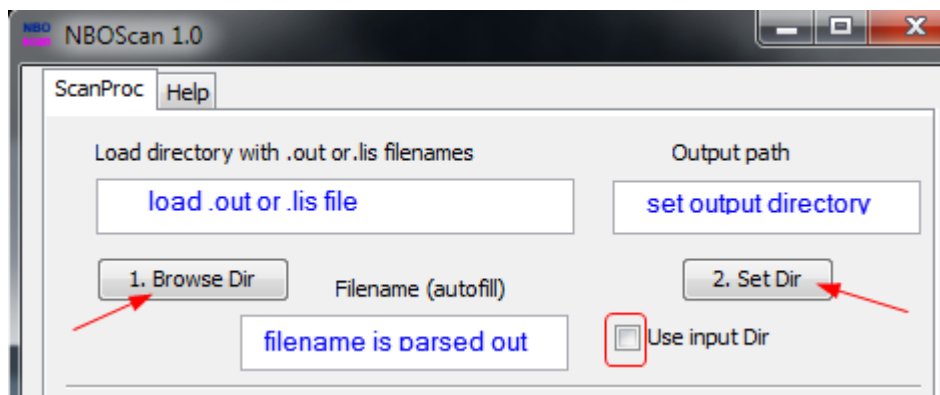
Figure 3

Next, set parameters for the single point energy calculation in the **section 3** (**Figure 4**). Those include the level of theory, basis set (pull-down menus) and additional comments and keywords to the route card. Alternatively, type in the custom level of theory and basis set.
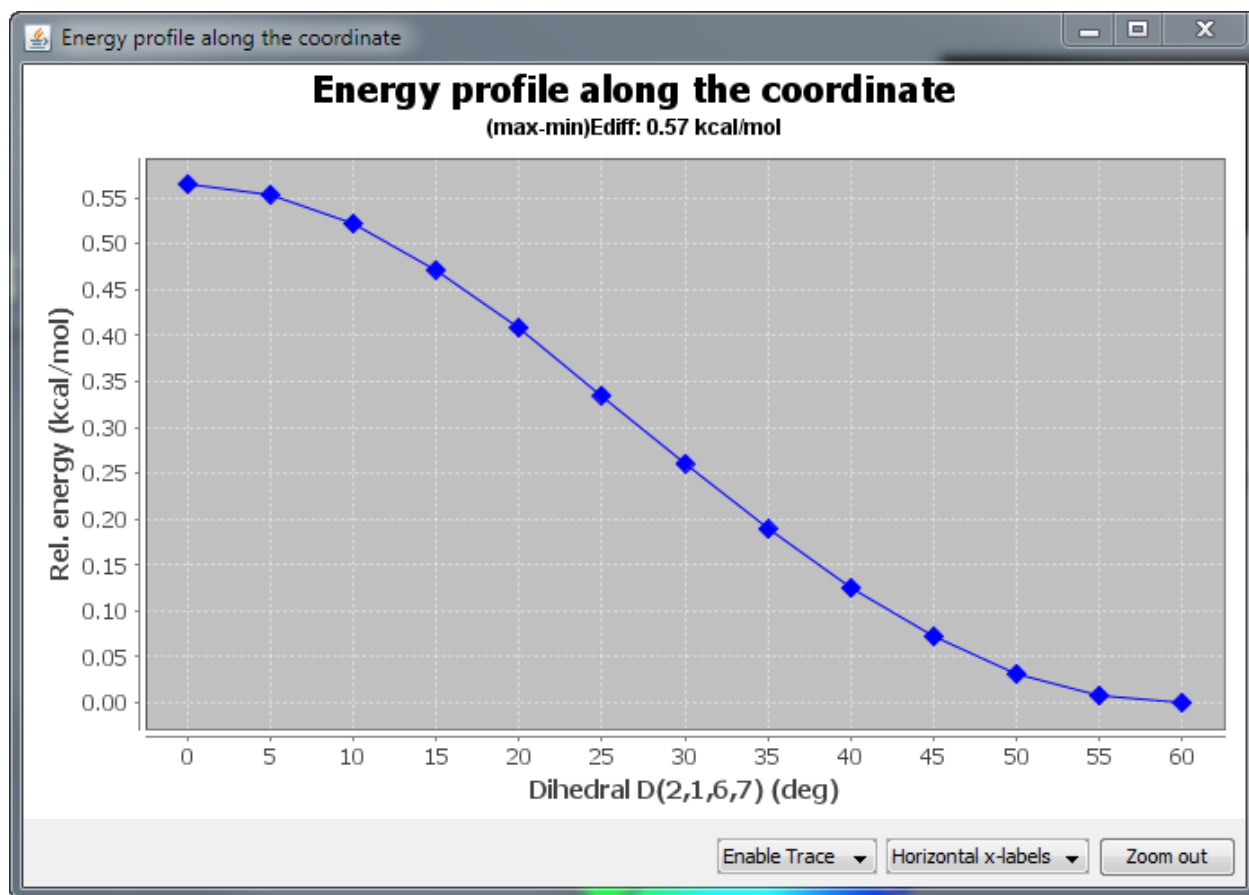

Figure 4

Optionally, check the Plot profile box to output the energy profile along the scanned coordinate. This will plot the total electronic energies at different dihedral angles (0-60 deg) (**Figure 5**).

Enable/disable additional options at the bottom of the window. Energy values at calculated points can be retrieved by pointing the mouse at the blue diamond. Axis values can be toggled between horizontal/vertical.

Figure 5

Section 4 involves entering NBO keywords or selecting the preset NBO properties (**Figure 6**). For more complex keyword lists, use the GennboHelper application described earlier and
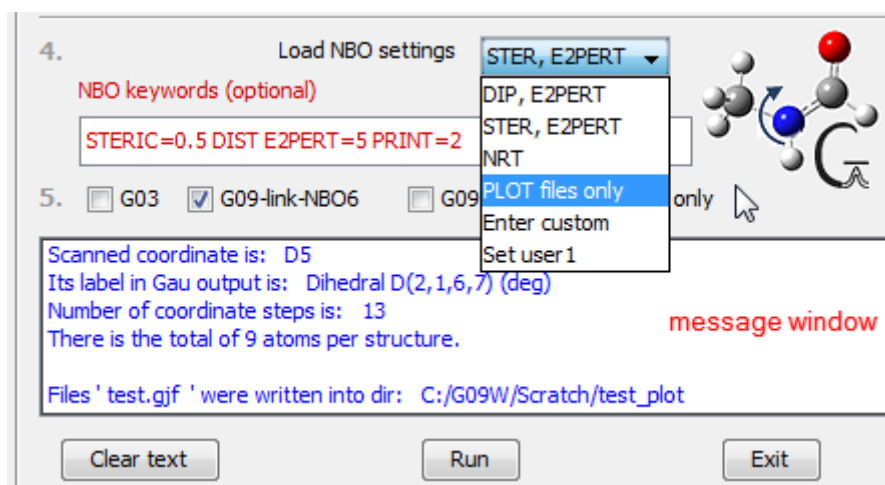
Figure 6

the Enter custom keywords. The latest version of the GennboHelper can be downloaded from the http://www.marcelpatek.com/nbo/nbo.html#gennbohelper.

Choosing the **PLOT files only** option will generate the corresponding NBO keywords necessary to create PLOT files for each scanned geometry. The last option, **Set user 1**, allows entering custom keywords that are retrieved next time when running the application.

Instructions to Gaussian program on how to perform NBO calculations are selected on **line 5**.

- G03 option uses older NBO3 module compiled as part of Gaussian 03 package.
- G09-link-NBO6 option adds keywords "EXTERNAL" and "pop=nbo6read" into the G09w route card and links NBO6 Windows binaries to G09w (revision D.01) [**DEFAULT**]. This option requires having gaunbo6.bat file (part of the NBO6 package) in the main Gaussian directory (e.g., C:\G09W\gaunbo6.bat).
- G09-NBO option adds NBO6 specific keywords (pop=nbo6read) into the route card of G09w, which had NBO6 compiled together with G09w binaries.
- .47 file only option instructs ESS to generate .47 archive file for later analysis by GENNBO5/6. This is equivalent to NBO keywords ARCHIVE FILE=xxx.

The message window at the bottom (**Figure 6**) provides information related to the key scan parameters, such as, name of the scanned coordinate, its description in the output file, number of extracted geometries, and total number of atoms in the molecule. Path to files created by NboScan application is also part of the output.

To facilitate the next step, that is, evaluation of each geometry with specified NBO keywords,
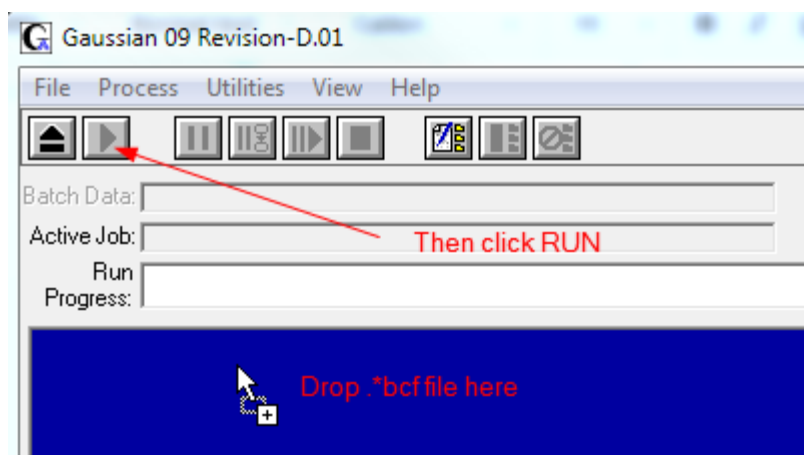
Figure7

Gaussian batch file (*.bcf) is created at the end of the run. Just drop the batch file into the main Gaussian09w window and click the "run" triangle icon (**Figure 7**).

Files created after the run are shown in **Figure 8**. Each created file has a suffix indicating value of the scanned coordinate.
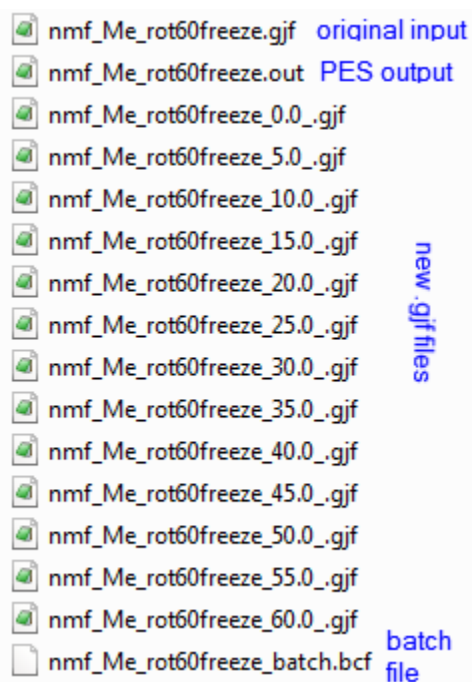
Figure 8

3.0 NBOScan Usage – Details

3.1 Settings

After the first run, NBOScan will create file **nboscan_settings.xml**, which keeps the last entered path to .out file, filename and path to output directory on your computer. Also, if you have entered additional comments or NBO custom settings (Set user1), values will be stored and retrieved at each run. Path to nboscan_settings.xml file is the same as the path of main NboScan.jar file (e.g., c:\nbo\NboScan). This file can be easily edited and individual entries changed manually (**Figure 9**).

```xml
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<settings>
    <id1>F:/Computation/Gaussian03/Examples/Scans/NMR_Me_rotation</id1>
    <id2>nmf_Me_rot60freeze</id2>
    <id3>F:/Computation/Gaussian03/Examples/Scans/NMR_Me_rotation</id3>
    <id4>Test run</id4>
    <id5>NBCP</id5>
    <id6>NBCP</id6>
    <id7></id7>
</settings>
```

Figure 9

4.0 Updates

To check for the current version of NBOScan, locate the version at the top-left of the main application window. In this case, it is version 1.0 (**Figure 10**).
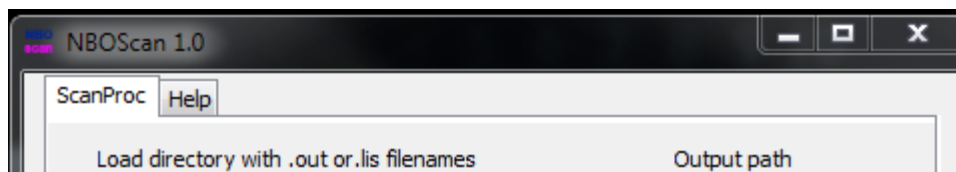
Figure 10

To get the latest version, click the link at the bottom of the main application or visit NBO Scripts and Handy Applications webpage. Download the latest version, and replace files in the original directory (c:/nbo/NboScan).