DP4+ App

https://github.com/Sarotti-Lab/DP4plus-App

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Example Manual - DP4+
(NMR – Gibbs freq)

Overview

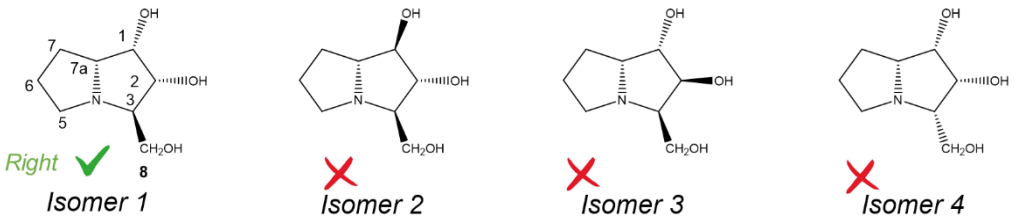
The DP4+App is designed to facilitate the correlation of experimental NMR chemical shifts with DFT magnetic tensors. *This manual outlines the process of performing DP4+ calculations using two separate Gaussian output files for a given conformer*. A key feature of the app is its ability to handle multi-level calculations, combining NMR tensors from one theory level with Boltzmann weighting derived from energies at a different level.

This manual explains how to perform DP4+ probability calculations using two Gaussian output files for each conformer—one containing NMR tensor data and the other providing Gibbs free energy results. By adhering to these instructions, you can effectively apply the DP4+ methodology in your research.

Content

The "*example_nmr_gibbs*" folder contains the following components:

- *NMR calculations*: folder *nmr_log* stores 162 Gaussian outputs from the four depicted isomers. Previous structure optimization was carried out at the B3LYP/6-31G* level, followed by GIAO-DFT calculations using the command line:
  `# mpw1pw91/6-31+G** nmr scrf=(pcm,solvent=water)`
- *Energy calculations*: folder *energy_log* stores 162 Gaussian outputs from frequency calculation associated with each conformer. The calculations were performed with the command line:
  `# B3LYP/6-31G* opt(maxcycles=30) freq=noraman scrf=(pcm,solvent=water, smd,dovacuum)`
- *Correlation spreadsheet*: *Correlation Isom1.xlsx* comprises the experimental chemical shifts for the isomer 01 (the correct one). This file also incorporates correlation labels establishing a correspondence between experimental and computational data.



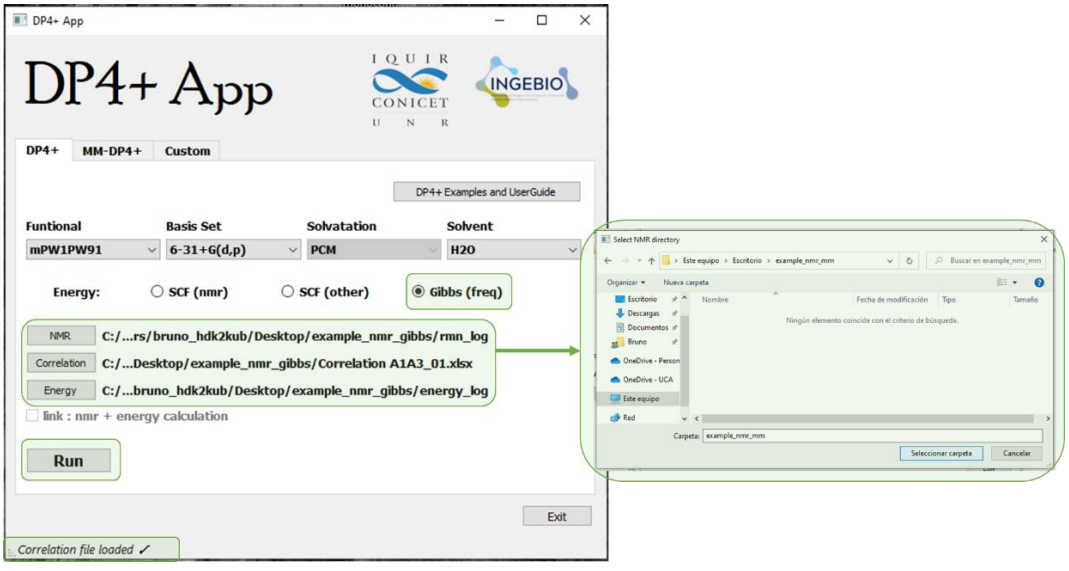
Procedure

To initiate the analysis, navigate to the DP4+ tab and configure the necessary parameters. The appropriate NMR theory level is as follows:

- ***Functional***: mPW1PW91
- ***Basis set***: 6-31+G (d,p)
- ***Solvatation***: PCM
- ***Solvent***: H2O (water)

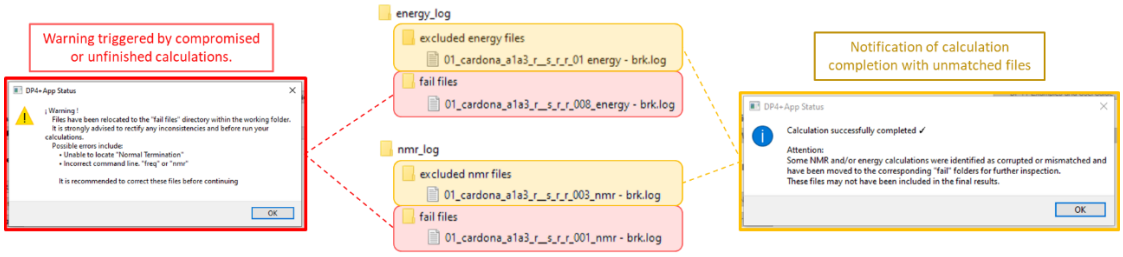
To proceed, tick the **SCF (other)** or **Gibbs (freq)** button to enable the energy button and link check box. As the frequency calculations incorporate both SCF and Gibbs energies, either option is suitable. It is advisable to experiment with both and analyze the resulting differences.

Utilize the designated buttons situated beneath the theory level panel to select the folders and files in this example. DP4+App will validate the folders and correlation spreadsheet to ensure compatibility with the calculation. Please consult the User Manual's *'Warnings and Input Control*' section for specific requirements. The status bar will guide you through the procedure.

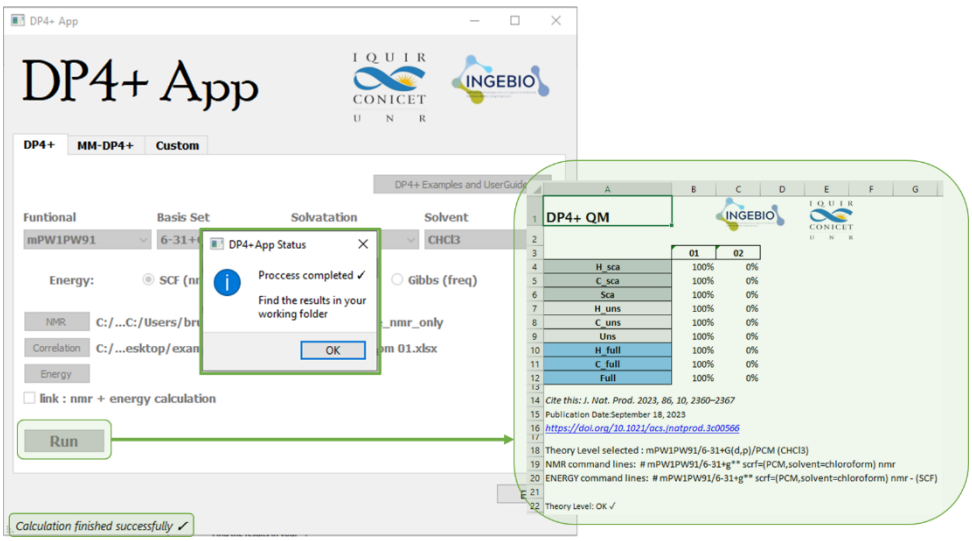


Once the configurations have been completed, the **'Run'** button will be enabled. Upon clicking it, the process starts by verifying the compatibility of the theory level and NMR command. In the event of an incompatibility, a warning will be issued. You may either proceed or return to modify the configurations.

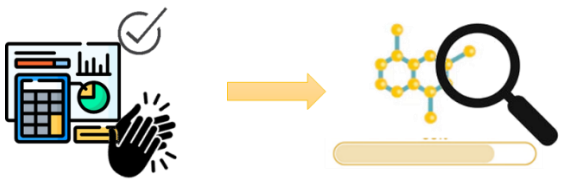
To simulate error conditions, corrupted files labeled *'brk'* have been introduced. These files are designed to generate alerts indicating damaged or mismatched data. DP4+App will isolate these files to facilitate uninterrupted calculations. In a real-world scenario, such calculations would require correction. Nevertheless, for the current demonstration, these alerts can be dismissed, and the affected files can be removed if wanted.



Once the process is finished, a pop-up will signal the successful termination of the DP4+ calculation, and the results will be automatically displayed. If the broken sample files have been removed, the notification should resemble the following image.



The computed data will be stored in the file *'DP4plus_results.xlsx'* located in the working directory. The calculation is now finished, allowing you to begin your analysis.



Disclaimer

This example is provided for educational purposes only to illustrate the application's capabilities. The analysis is not based on real-world data. To simplify distribution, not all conformations within a 10 kcal/mol energy window are included in this example. Therefore, replicating this study may produce varying outcomes.