DP4+ App

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

sarotti@iquir-conicet.gov.ar

Example Manual - DP4+
(NMR - link - SCF energy)

Overview

The DP4+App is designed to facilitate the correlation of experimental NMR chemical shifts with DFT magnetic tensors. *This manual provides step-by-step guidance on performing DP4+ calculations with linked Gaussian output files*. 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 focuses on performing DP4+ probability calculations utilizing Gaussian output files generated with link setup. These output files encompass both NMR and single-point energy data. By following the outlined procedures, you will be able to effectively apply the DP4+ methodology to your research.

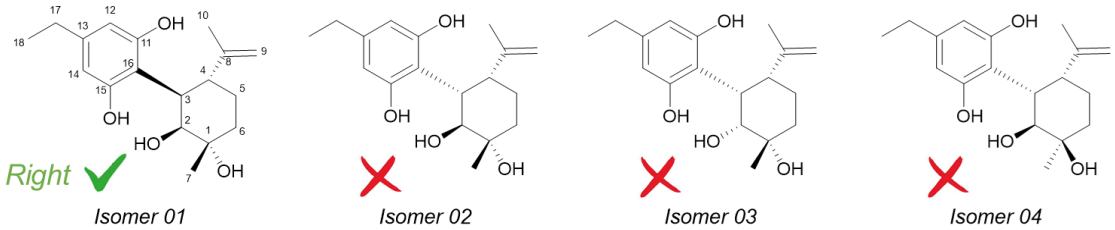
Content

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

- *Gaussian calculations*: Forty-two '.log' files provide NMR and single-point energy data for the four depicted isomers. Previous structure optimization was carried out at the B3LYP/6-31G* level, followed by linked calculations using the Gaussian 09 commands:

```
# mpw1pw91/6-31+G** nmr scrf=(pcm,solvent=water)
--link1--
# B3LYP/6-31+G** geom=allcheck test scrf=(pcm,solvent=water,smd,dovacuum)
```

- *Correlation spreadsheet*: 0_*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.

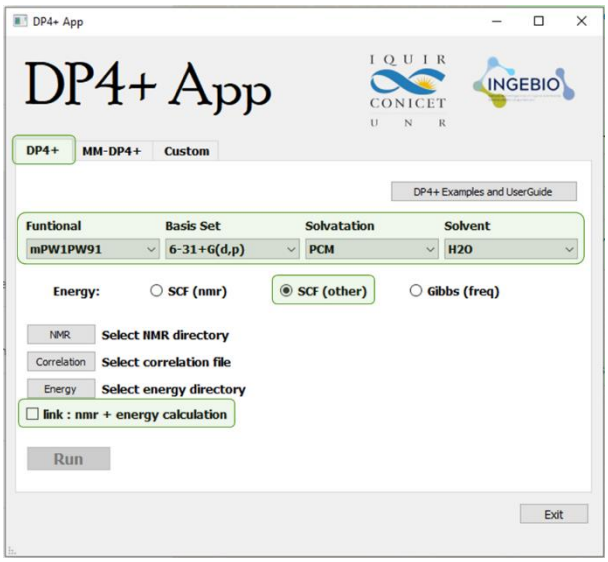


Procedure

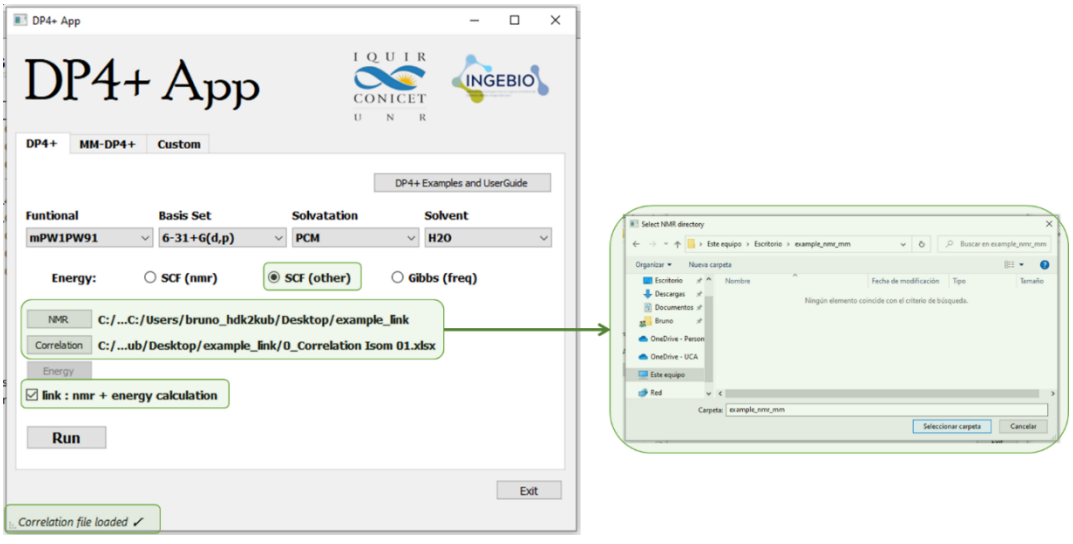
To initiate the analysis, navigate to the DP4+ tab and configure the necessary parameters. The appropriate NMR theory level is as follows:

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

Check the '**SCF (other)**' option to enable energy selection and link checkbox. The Gaussian files in this example do not include frequency calculations, therefore using the '**Gibbs (freq)**' option will result in process termination. Only SCF energies can be utilized, either from the NMR calculation itself (**SCF (nmr)**) or through a link.



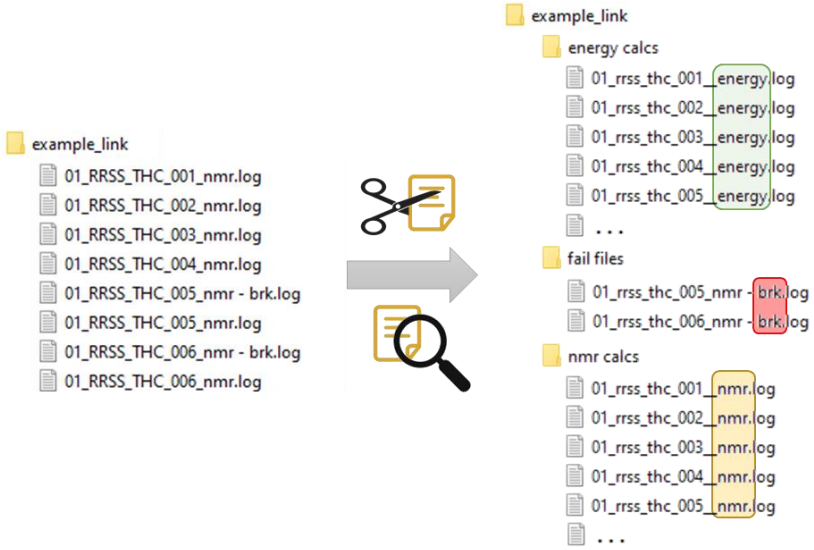
Utilize the designated buttons situated beneath the theory level panel to select the folders and files in this example. DP4+App will validate the folders and correlation spreadsheet to ensure compatibility with the calculation. Please consult the User Manual's *'Warnings and Input Control*' section for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



For this specific case, check the '☐ **link: nmr + energy calculations**' box and disable the '**Energy**' selection button. This will setup the use of shielding tensors from the NMR calculations and the Boltzmann weighting with the single point calculation.

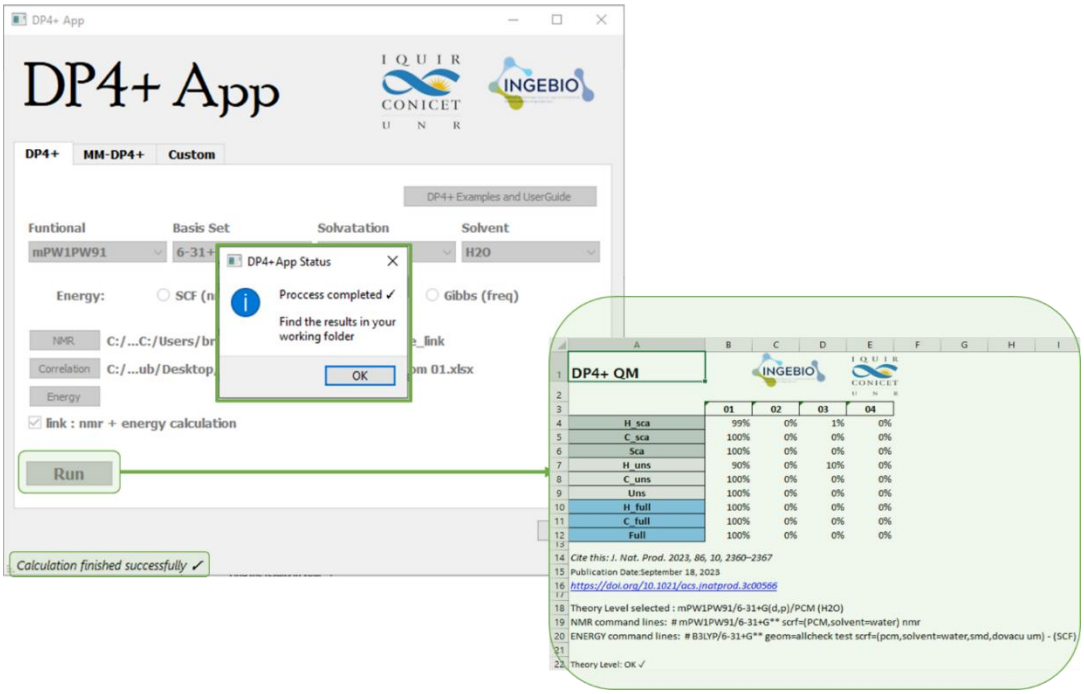
Once the configurations have been completed, the **'Run'** button will be activated. Upon clicking it, the process starts by verifying the compatibility of the theory level and NMR command. In the event of an incompatibility, a warning will be issued. You may either proceed or return to modify the configurations.

Subsequently, the NMR and energy calculations will be separated, generating the folders *'energy_calcs'* and *'nmr_calcs'*. Additionally, file integrity will be assessed. Files that are broken or have an incorrect NMR + energy link will be moved to the '*fail_files'* folder.

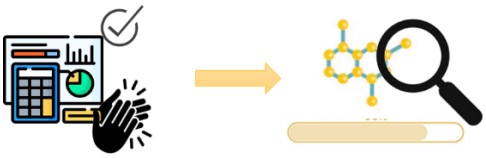


To simulate error conditions, corrupted files labeled *'brk'* have been introduced. These files are designed to generate alerts indicating damaged or mismatched data. DP4+App will isolate these files to facilitate uninterrupted calculations. In a real-world scenario, such calculations would require correction. 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.