DP4+ App

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

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Example Manual - MM-DP4+

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 **MM-DP4+** calculations.*

This manual focuses on performing MM-DP4+ probability calculations utilizing single Gaussian output files coming from NMR calculations. The data subtracted from these will be the shielding tensors and the SCF energy at the given theory level. By following the outlined procedures, you will be able to effectively apply the DP4+ methodology to your research.

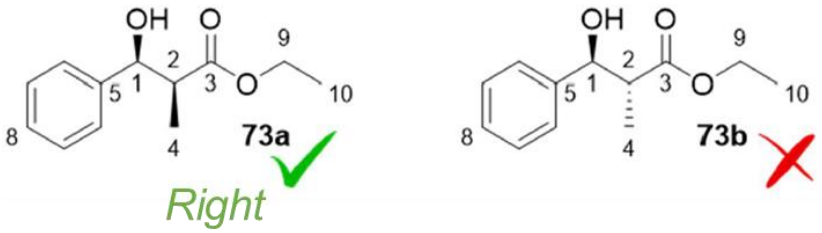
Procedure

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

- *Gaussian calculations*: Seventy-six '*.log*' files provide NMR calculations for the depicted isomers. Previous structure optimization was carried out at the B3LYP/6-31G* level, followed by calculations using the Gaussian 09 commands:

```
# wb97xd/6-31+g** scrf=(pcm,solvent=chloroform,smd,dovacuum) nmr
```

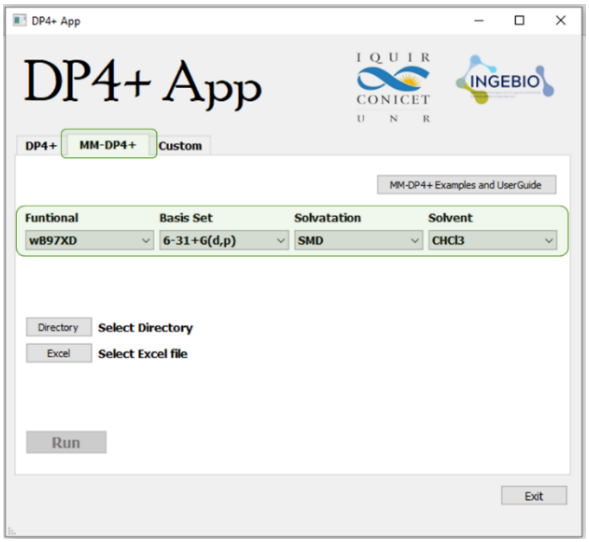
- *Correlation spreadsheet*: *73a - correlation file.xlsx* comprises the experimental *chemical* shifts for isomer 73a (the correct one). This file also incorporates correlation labels establishing a correspondence between experimental and computational data.



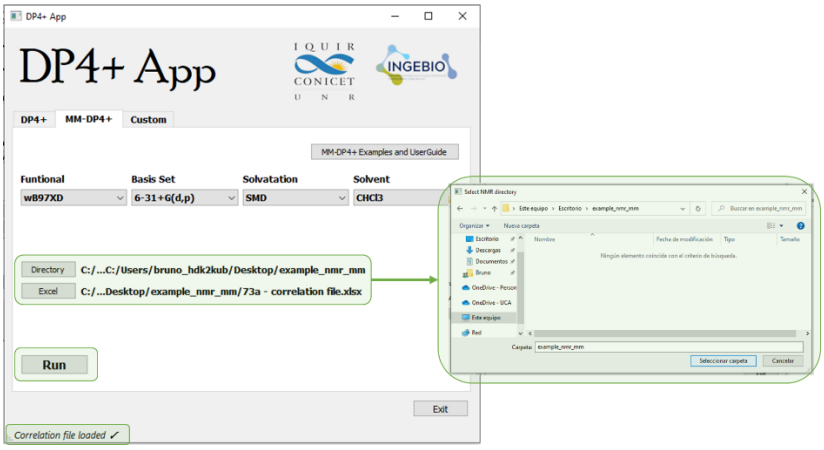
Procedure

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

- ***Functional***: wB97XD
- ***Basis set***: 6-31+G (d,p)
- ***Solvatation***: SMD
- ***Solvent***: CHCl3

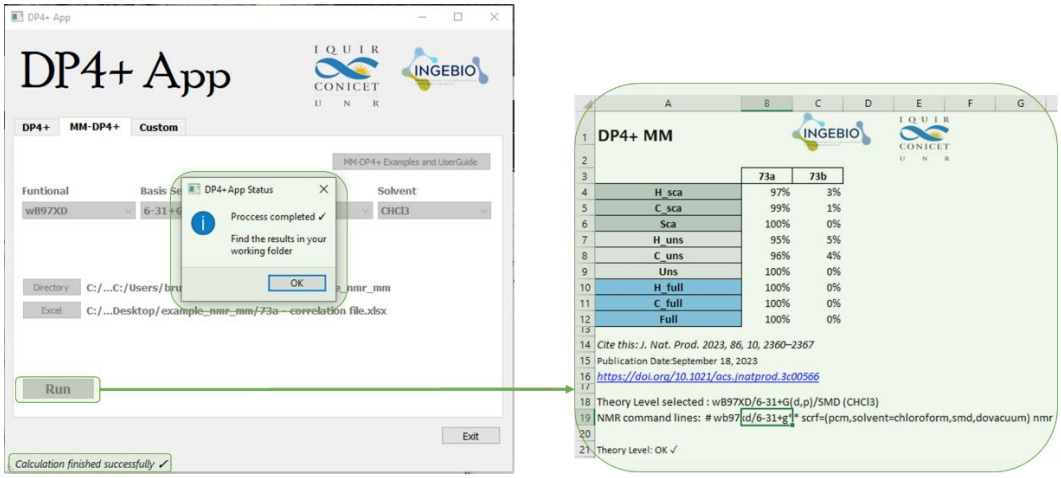


Utilize the designated buttons situated beneath the theory level panel to select the folders and files in this example. DP4+App will validate the folders and correlation spreadsheet to ensure compatibility with the calculation. Please consult the User Manual's *'Warnings and Input Control*' section for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

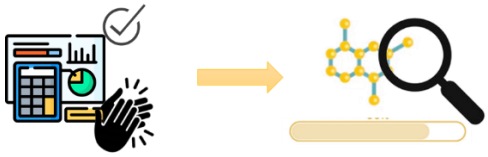


To simulate error conditions, corrupted files labeled *'brk'* have been introduced. These files are designed to generate alerts indicating damaged or mismatched data. DP4+App will isolate these files to facilitate uninterrupted calculations. In a real-world scenario, such calculations would require correction.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

Once the 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.



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.



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.