DP4+ App

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

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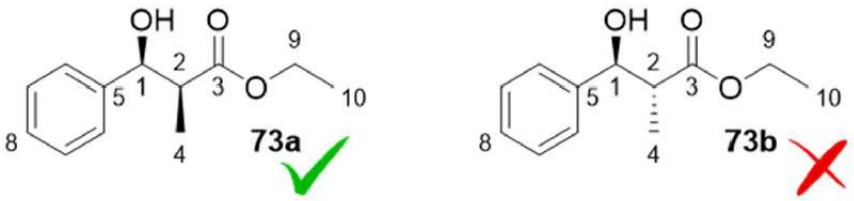
Example Manual

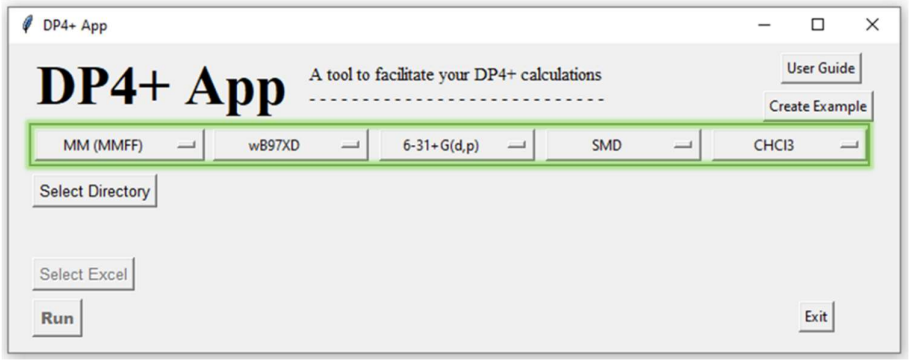
The folder named 'nmr_examples', which houses this file, also encompasses the following elements:

- *Gaussian calculations*: There are 33 and 42 files for the isomers 73a and 73b, respectively. These structures were optimized with MMFF force field and the calculations were performed with GIAO-DFT using the command line: #wb97xd/6-31-g" scrf (pcm,solvent-chloroform,smd,dovacuum) rmr
- *Experimental and correlation spreadsheet*: This file comprises the experimental chemical shifts for the 73a isomer (the correct one), along with the correlation labels connecting the experimental data to the in silico models In this instance, a single set of labels is employed for all conformers.

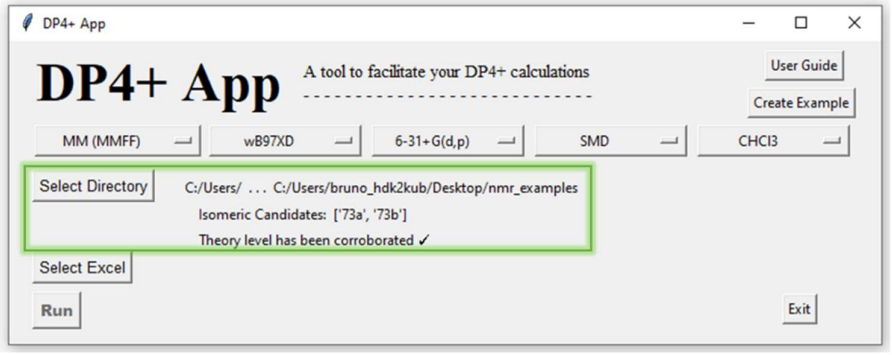


For the analysis of this system, the correct parameters are:

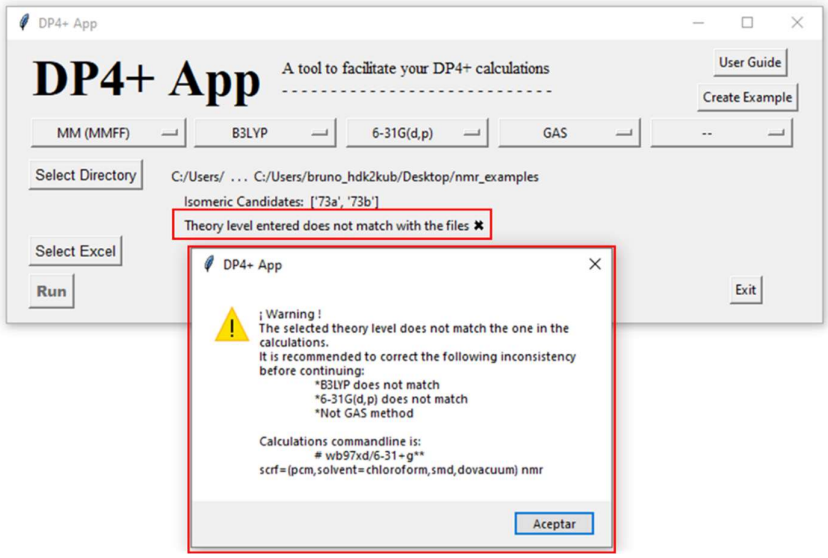
- *Mode*: MM (MMFF), indicating MM-DP4+ calculation
- *Functional*: wB97XD
- *Basis set*: 6-31+G (d,p)
- *Solvatation*: SMD
- *Solvent*: CHCl3



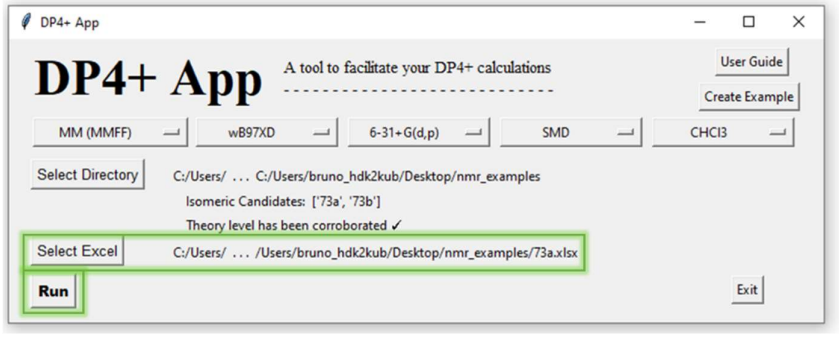
Next, choose the "nmr_example" folder. The DP4+ App will then proceed to validate that the selected theory level aligns with the files provided.



If incorrect parameters are chosen, a popup will appear, offering instructions on how to rectify the selection. For instance, if the chosen parameters are: MM (MMFF), B3LYP, 6- 31G(dp), GAS, the following warning message will be displayed. However, it's important to note that this alert does not prevent you from proceeding with the calculation if you decide to continue with the current selection.



Afterward, proceed to select the '73a' worksheet and press the "**Run**" button.



Once the calculation is completed, the results spreadsheet will open automatically, and a notification will pop up, indicating that the process has concluded.