# Theoretical Investigation on $^{13}C$ and $^{1}H$ NMR Chemical Shifts and Molecular Structure of an Limonoid from *Swietenia macropylla*

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Limonoids represent a group of chemically related triterpenes found in *Switenia macrophylla*. Limonoids have been found to have anti-carcinogenic activity [1] and activity against insects.[2] The objective of this work was to support the interpretation of experimental data concerning the stereochemistry and molecular structure of one limonoid (**Figure 1**). All ab initio quantum calculations were performed on ORCA suite of programs at B3PW91/DGAUSS level of theory. The linear regressions concerning theoretical and experimental data are show in **Figure 2.**

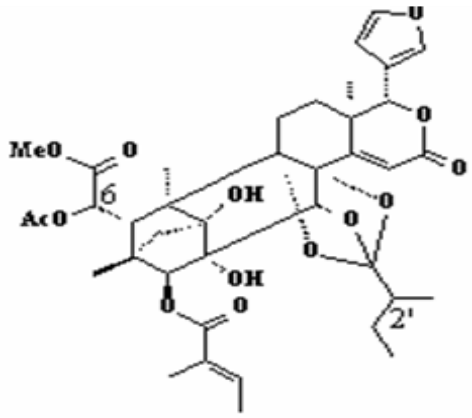


**Figure 1:** Struture of limonid.

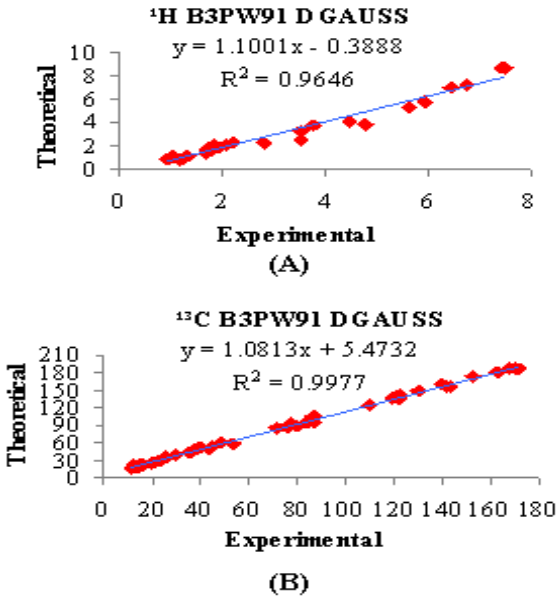


**Figura 2**. Correlation between experimental and theoretical NMR data: (A) δH and (B) δC.

Our results show very good agreement between theoretical and experimental data[3] and suggest that this limonoid should have a R-stereochemistry in the 6 and 2'positions.

Keywords: DFT, B3PW91, DGAUSS, limonoids.

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