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## Very fast and surprisingly accurate GIAO-mPW1PW91/3-21G//PM7 scaling factor for <sup>13</sup>C NMR chemical shifts calculation

Fabio Luiz Paranhos Costa  
Federal University of Goias, Brazil

In this work, we present a new GIAO-HDFT universal scaling factor (mPW1PW91/3-21G//PM7(I)) and a comparative study in which is investigated its ability to predict NMR <sup>13</sup>C chemical shifts ( $\delta$ ) with high cost-effectiveness ratio. A set of 22 small molecules providing 27 different <sup>13</sup>C  $\delta$  determined in the gas phase was used for all scaling factors protocols: B3PW91/cc-pVDZ//B3PW91/cc-pVDZ (II), B3PW91/cc-pVTZ//B3PW91/cc-pVDZ (III), B3LYP/6-311+(2d,p)//B3LYP/6-31G(d) (IV), mPW1PW91/6-31G(d)//PM7(V), mPW1PW91/6-31G(d)//mPW1PW91/6-31G(d) (VI). Despite the calculation approximations the  $\delta$  calculated at the GIAO-mPW1PW91/3-21G//PM7 using a simple relationship ( $\delta_{\text{scal}} = 1.14 \cdot \delta_{\text{calc}} - 4.7$ , where  $\delta_{\text{calc}}$  and  $\delta_{\text{scal}}$  are the calculated and the linearly scaled values of the <sup>13</sup>C  $\delta$ , respectively) were able to yield MAD and RMS errors as small as those obtained with other GIAO-HDFT with bigger basis sets (protocols (II) to (VI)). The robustness of the new protocol and its applicability to practical problems was evaluated by the calculation of the  $\delta$  for two natural compounds with synthesis, biological and therapeutic interest: tryptanthrin (indolo[2,1-b]quinazoline-6,12-dione) and (-)- loliolide (7aR)-6-hydroxy-4,4,7a-trimethyl-6,7-dihydro-5H-1-benzofuran-2-one. For both compound, the 6 protocols presented good agreement with experimental data. Moreover, for the second compound, the new protocol performs even better than the 5 others. In conclusion, GIAOmPW1PW91/3-21G//PM7 linear regression obtained by using the experimental and the calculated data, is a very attractive tool as an alternative to more computationally demanding approaches, which are usually applied in order to achieve <sup>13</sup>C NMR  $\delta$  calculations.

### Biography

Fabio Luiz Paranhos Costa has completed his PhD from University Federal of Rio de Janeiro and Postdoctoral studies from University Federal Fluminense. He has published more than 20 papers in reputed journals.

fabbioquimica@gmail.com

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