Approximate Reduced Density Matrix for Bioactive Systems: an *ab-initio* Approach

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Modelling complex systems such as bioactive molecules in their real environment implies two notions : accuracy and robustness of the results, reasonable computation time. Usual ab initio methods or MD simulations do not fulfil those two conditions. Decreasing the computation time and keeping the reliability of an Hartree-Fock approach is possible through the 1-Particule Reduced Density Matrix which can be approximated as a sum of molecular fragments obtained from finite clusters simulating the local environment [1]. This method is a useful tool to go beyond the mere electrostatic properties and to obtain more precise and more sensitive information about interaction mechanisms and reactivity.

After its validation for simple periodic systems, the method was adapted and implemented for complex systems. We report our results obtained on some pharmaceutical compounds, such as busulphan and styrylquinolines.

[1] Ragot S, Gillet J.M., Becker P., *Physical Review B*, 2002, **65**, 235115.

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