A Molecular Orbital Study of the Conformational Properties of Cationic Ephedrine

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Ephedrine molecules shown in Figure 1 are expected to different conformations due to the flexibility of its ethanolamine side chain. But, ephedrine molecule has been much less thoroughly theoretical studied than phenethylamines such as dopamine, norepinephrine, phenethylamine, etc.[1-3] I have focus on the active sites of each conformers by using the properties derived from DFT, such as the E_{HOMO}, E_{LUMO}, energy gap, atomic charge, which have indicated the reactive behavior. Knowledge of the rotational potential for a ligand helps estimate the necessary minimum for a free energy decrease upon the formation of the ligand receptor complex. Theoretical values are even more important in cases such as these molecules and its receptors, where no experimental information is available regarding the structure of bioactive complex.

All calculations have been performed at the B3LYP/6-31G* level of theory by using Gaussian 03W[4] software package, B3LYP functional is a combination of Becke's three-parameter hybrid exchange functional[5] and the Lee-Yang-Parr correlation functional[6] which this combination of the ab initio method and basis set has been shown to be succesful in predicting the structures of similar molecules, with optimized geometries agreeing well with those available from experimental.

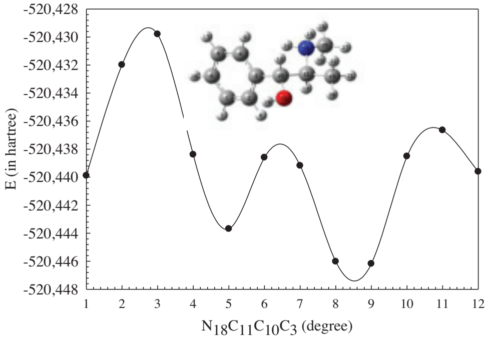

Figure 1. The selected rotational energy barrier profiles for cationic ephedrine

REFERENCES

[1] Alonso, J. L., Sanz, M.E., Lopez, J. C., Cortijo, V. *J. Am. Chem. Soc.* **131**, 4320-4326, 2009.
[2] Butz, P., Kroemer, R. T., Macleod, N. A., Robertson, E. G., Simons, J. P. *J. Phys. Chem. A*, **105**, 544-551, 2001.
[3] Butz, P., Kroemer, R. T., Macleod, N. A., Simons, J. P. *J. Phys. Chem. A*, **105,** 1050-1056, 2001.
[4] Gaussian 03, Rev. D 01 (Gaussian Inc, Wallingford CT) 2004.
[5] Becke, A. D. *J. Chem. Phys.* **98,** 1372-1377, 1993.
[6] Lee, C,. Yang, W., Parr, R. G. *Phys. Rev. B.* **37**, 785-789, 1998.