



SDI FINAL EVALUATION FORM 1.1

PART 1:

Journal Name:	American Chemical Science Journal
Manuscript Number:	2012_ACSJ_2905
Title of the Manuscript:	Theoretical Study of Stability, Tautomerism, Equilibrium Constants (pK_T) of 2-Thiouracil in Gas phase and Different solvents (water and Acetonitrile) by the Density Functional Theory Method

PART 2:

Editorial Comment:	Authors' Feedback:
In my opinion, the article should be published on the ACSJ with some important corrections. The main problem of this paper is that it presents only quantum calculations. Further it is unclear the novelty or the specific applications of the calculations reported, because some others authors have reported similar studies with other or the same theoretical general methods (Please, look at the references below). So, for considering the publication of this paper, the authors seems to have taken care most of the reviewer's comments, and especially include the usefulness of these results, or at least, the comparison of its results with experimental and/or theoretical information previously reported References: J. Am. Chem Soc. 1990, 112, 1504; J. Phys. Chem. B 2012, 116, 8793	Thank for your comments, in this paper we mainly calculated the molar transfer Gibbs energies of $\Delta\Delta G_i^0$ and inter conversion equilibrium constants are calculated. These calculations are first time we reported, so no literature values are available. Most of the authors are calculated only tautomers stability and equilibrium constant but we calculated in addition above two parameters are calculated. The results are useful for further researchers. This is my replay.