



## SDI FINAL EVALUATION FORM 1.1

### PART 1:

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| Journal Name:            | <a href="#">American Chemical Science Journal</a>                                                                                                                                                  |
| 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:

| FINAL EVALUATOR'S comments on revised paper (if any)                                                                                                                                                                                                                                                                                                                                                   | Authors' response to final evaluator's comments                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
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| <p>My main comment on the first version was that only calculated numbers are reported, which is pretty standard and can be done on any PC for this kind of calculations nowadays, and that comparison with experiment is failing.</p> <p>Now the author replied that no experimental data are available. Thus we have just numbers, the true meaningfulness of which cannot be judge by any means.</p> | <p>Ok, I accept your comment, but most of the computational chemistry research papers are not include the experimental values, if available the values to include, But some of the chemical properties are not calculated by experimentally, at that time where we are getting the experimental values. If all the computational calculations want to experimental values always, what is the need of the computational calculations and software's?</p> <p>The Reviewer comment is just the data is numbers, even experimental values also just numbers, what is the difference I don't know.</p> <p>The DFT and it basis set getting Nobel prize which is the standard for the programme.</p> <p>This the my replay,</p> |