RELATIVE STABILITY OF CONFORMERS IN SOLUTION WITH COSMO-RS

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The ability of the COSMO-RS method to predict the relative stability of different conformers of the same species in solution was evaluated by comparing computational results with experimental conformer data for 105 molecules from 20 literature sources [1]. Various solvents were used ranging from $CDCl_3$, CD_2Cl_2, benzene, toluene, ethyl ether, tetrahydrofuran, acetone, dimethylformamide, DMSO (and DMSO-d_6), water and ethanol. The solvent choice was dictated by the solvents used in the literature. In the case of 16 molecules the experimental quantitative conformer abundances were also available and were compared with computational data. The results show that although COSMO-RS cannot accurately reproduce the conformer abundances, the most stable conformer is determined correctly in 103 cases out of 105. This result validates the use of COSMO-RS in several applications (e.g. distribution coefficients, vapor pressures, solubilities) where the most stable conformer of a molecule can be different in different phases and meaningful results cannot be obtained with incorrect predictions of the most stable conformer.

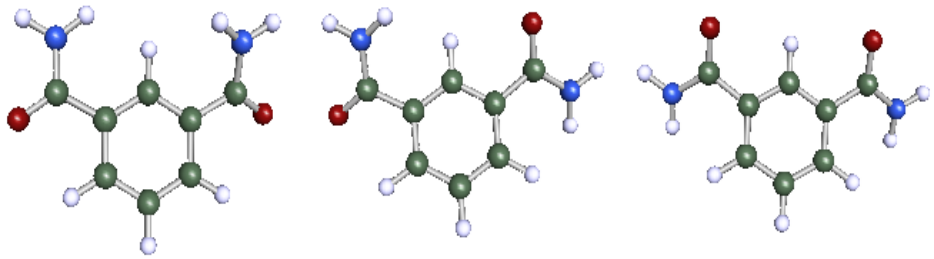

Figure 1. An example of studied conformers for the molecule of 1,3-benzenedicarboxamide[1]

References

1. Pung, A.; Leito, I. Predicting Relative Stability of Conformers in Solution with COSMO-RS. J. Phys. Chem. A, 2017, 121 (36), pp 6823–6829

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