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Characterization of metformin/functional groups associates in aqueous system

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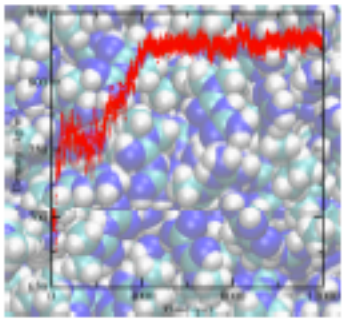
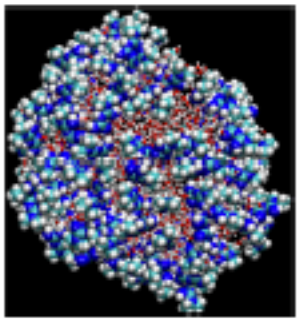
In this contribution we present a fundamental study of metformin (*N,N*-dimethylimidodicarbonimidic diamide) aqueous mixtures, with three different functional groups, specifically, acetic acid, ethanol and DABCO (1,4-diazabicyclo[2.2.2]octane). The chemical equilibrium and thermodynamic parameters were determined by molecular dynamics in the NpT and NVT ensembles at standard conditions using GROMACS [1]. All the molecular models were TraPPE-like built [2]. The outcomes of this study, particularly, the prediction of the free energy of binding for metformin/functional group and the insights on the solvent effect over this parameter will help the designing process of novel functionalized activated carbon for metformin recovery from water [3].





Left) Calculated metformin density 928.59± (7.26935) kg/m^3 at 25 °C and 1 atm. Right) Water metformin micelle same conditions.

[1] Lindahl, E.; Hess, B.; van der Spoel, D. J. Mol. Model. 2001, 7, 306.

[2] Sokkalingam, N.; Kamath, G.; Cosciona, M.; Potoff, J.J. J. Phys. Chem. B 2009, 113, 10292.

[3] AL-Bayati, R.A. European Journal of Scientific Research ISSN 1450-216X Vol.40 No.4 (2010), pp.580-588