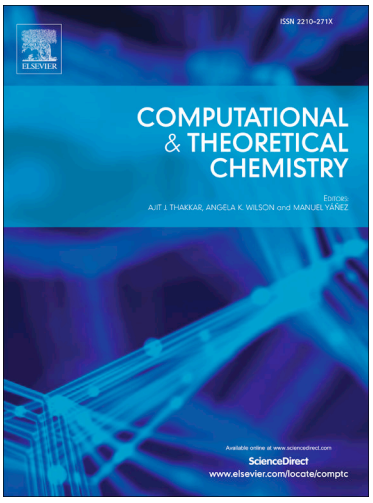

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Structural and energetic quantum chemical investigations into how the bioactive thiazolidinedione and rhodanine scaffolds interact with cytosine to form part of DNA

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Abstract

The interaction within biologically active complex configurations composed of thiazolidinedione - cytosine (TC) and rhodanine-cytosine (RC) have been fully investigated using B3LYP and M062X methods in conjunction with various basis sets, including 6-311++G(d,p), 6-311++G(2d,2p), 6-311++G(df,pd) and AUG-cc-pVDZ. Dispersion corrections to interaction energies using M06-2X-GD3 and double hybrid density functionals (B2PLYP-GD2, B2PLYP-GD3 and mPW2PLYP-GD2) have also been taken into account. The results showed that the interaction energies, including long range dispersion corrections obtained using double hybrid density functionals, are about 1 - 2.5 kcal/mol higher than uncorrected ones. Various combinations of all possible sites around the monomers which could lead to formation of stable complex configurations were considered, and then six double hydrogen bonded interactions which are formed in a cyclic pattern were further investigated for both complex configurations between cytosine-thiazolidinedione and cytosine-rhodanine. The intermolecular hydrogen bonds which are involved in forming of cyclic interaction patterns are of NH---O(N) and CH---O(N) types.

The TCS′2S1 and RCS′2S1 complex configurations were found to have the largest interaction energies within all the complex configurations studied for cytosine-thiazolidinedione and cytosine-