

Theoretical study on the anomeric, exo-anomeric and reverse anomeric

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Abstract: The anomeric effect is well known, but its origin is still controversial, since electrostatic and electron delocalization interactions are invoked to explain the stereochemical preferences of α -substituted tetrahydropyrans. In cases where both endocyclic and exocyclic heteroatoms bearing electron lone pairs take place, the exoanomeric effect can appear, in addition to the classical anomeric effect. In order to further explore these effects as stabilizing interactions of the conformations of sixmembered rings, the present work evaluated a series of heterocyclic compounds substituted at C2 by various groups [F, NH2, NH(CH3), OH, OCH3, N(CH3)2]. Calculations were carried out at the ω B97XD-6-311++g(d,p) level, using the Gaussian 09 program. The geometries for the stable conformers were fully optimized in the gas phase and implicit DMSO (using the polarizable continuum model). Subsequently, natural bond orbital (NBO) analysis was also performed; finally, NMR and AIM parameters were calculated in order to assess the interactions responsible for the titled effects. The theoretical calculations allowed to conclude that molecules containing an exocyclic nitrogen show the reverse anomeric effect, while the structures with a fluorine at C-2 and an endocyclic oxygen show the anomeric effect. On the other hand, structures with the fluorine substituent at C-2 and nitrogen as endocyclic atom show the reverse anomeric effect. For molecules containing endocyclic nitrogen and exocyclic oxygen atoms only, the normal anomeric effect takes place. The most important contribution to the effects studied in this work was the classical one. The calculations indicated some structures that induce the reverse anomeric effect.

Key-words: Anomeric effect, exo-anomeric effect, theoretical calculations, Perlin effect **Support:** This work has been supported by Federal university of Lavras **References:**

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