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SUPPLEMENTARY MATERIAL TO

# Unveiling the regioselective synthesis of antiviral 5-isoxazol-5-yl-2'-deoxyuridines from the perspective of a molecular electron density theory

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## COMPUTATIONAL METHODS

Recent studies on polar and non-polar cycloaddition reactions have allowed selecting the MPWB1K[1] functions in conjunction with the 6-311G(d,p)[2] as the most adequate computational model to study 32CA reactions and has been consequently applied in the present MEDT study. The Berny analytical gradient optimization method[3] was used for the optimizations and the stationary points were characterized by frequency calculations verifying the absence of imaginary frequency for the minima and TSs with one imaginary frequency. The energy profile connecting the TS and the associated minima was verified from the Intrinsic Reaction Coordinate (IRC)[4] calculations using the second order González–Schlegel integration method.[5,6] Solvents effects in toluene, THF, dichloroethane, acetonitrile, DMSO and water were studied by optimizing the structures in the respective solvents using the polarizable continuum model (PCM)[7,8] within the self-consistent reaction field (SCRF)[9–11] framework at PCM/ /MPWB1K/6-311G(d,p) level of theory. The thermodynamic calculations were performed at 298 K and 101.325 kPa pressure. Natural population analysis (NPA)[12,13] was performed at the TSs to calculate the GEDT[11] from the sum of natural atomic charges ($q$) at each framework ($f$) using the formula GEDT:

$$(f) = \sum_{q \in f} q \qquad (1)$$

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where the positive GEDT denotes transfer of electron density from the considered framework. The CDFTindices[12,13] were calculated from the standard equations reviewed in Reference 14. All calculations were performed using the Gaussian 16 suite of programs.[14] The topological analysis of the ELF and the AIM and the IGMH calculations were realized using Multiwfn[15] software. The ELF isosurfaces were visualized using UCSF Chimera[16] software, and the IGMH isosurfaces were visualized by VMD software.[17]

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