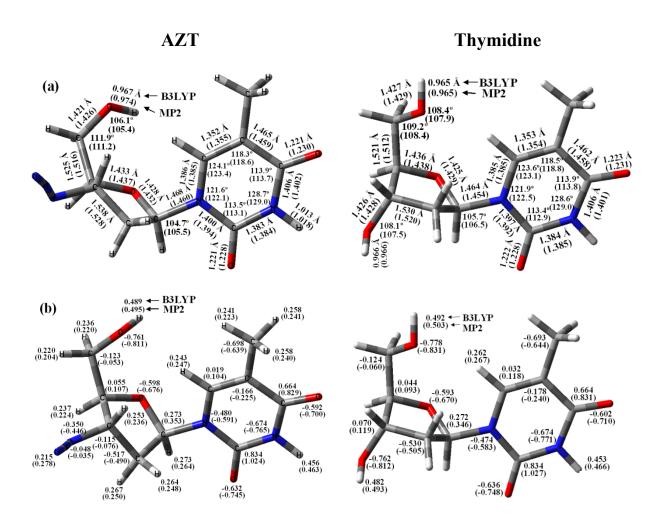
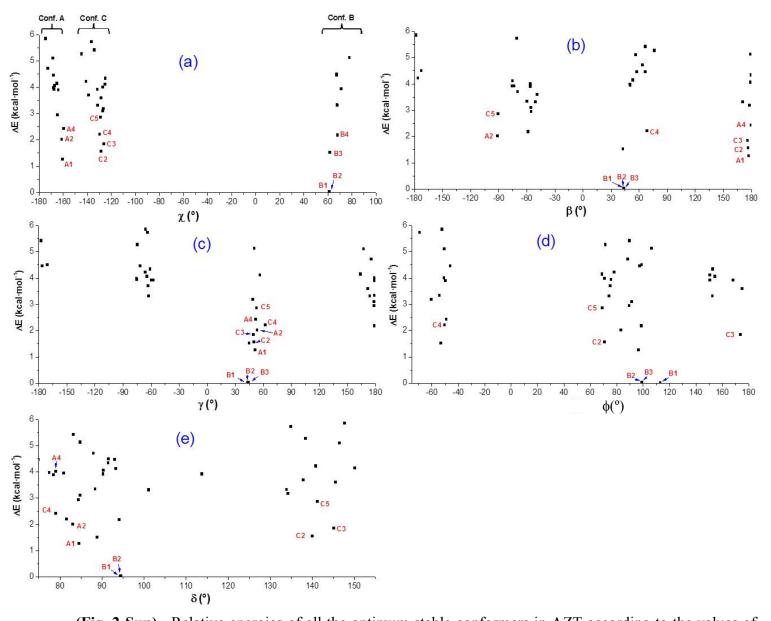
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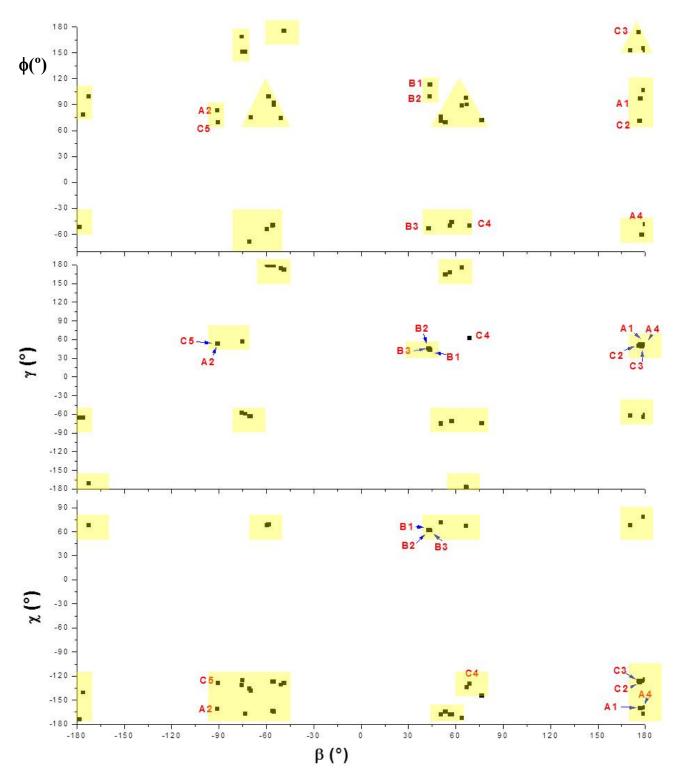
## SUPPLEMENTARY MATERIAL



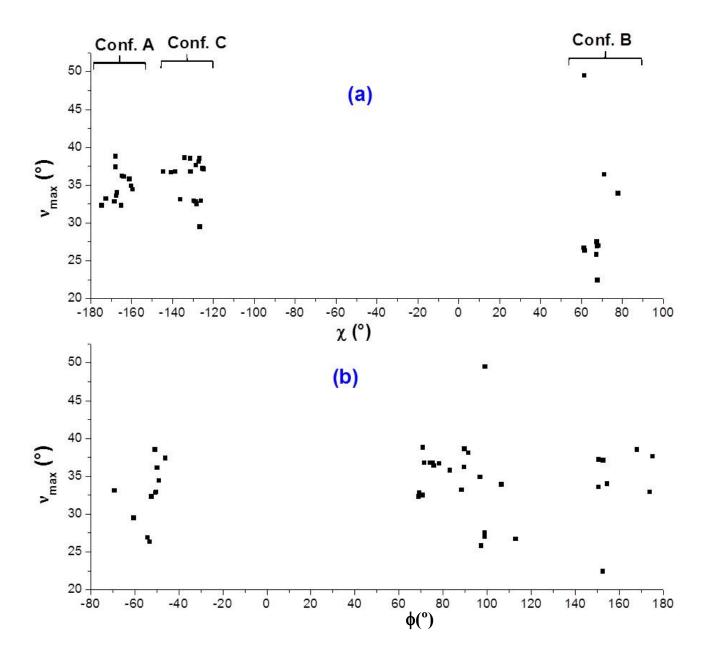
**(Fig. 1-Sup).** Differences between the conformer C1 of AZT and dT: (a) in the bond lengths, (b) in the NBO atomic charges.



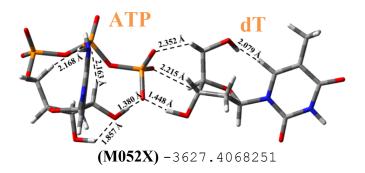
(Fig. 2-Sup). Relative energies of all the optimum stable conformers in AZT according to the values of the five exocyclic torsional angles:  $\chi$ ,  $\beta$ ,  $\gamma$ ,  $\phi$ , and  $\delta$ .



(Fig. 3-Sup). Distribution of all the optimum conformers according to the values of the exocyclic torsional angles  $\phi$ ,  $\gamma$  and  $\chi$  versus  $\beta$ . The stability areas of the conformers are marked in yellow colour.



(Fig. 4-Sup). Distribution of all the conformers according to the values of the exocyclic torsional angles  $\chi$  and  $\phi$  versus  $\nu_{max}$ .



(Fig. 5-Sup). An inadequate orientation of the ATP-dT interaction doesn't lead to a rotation of H5'.