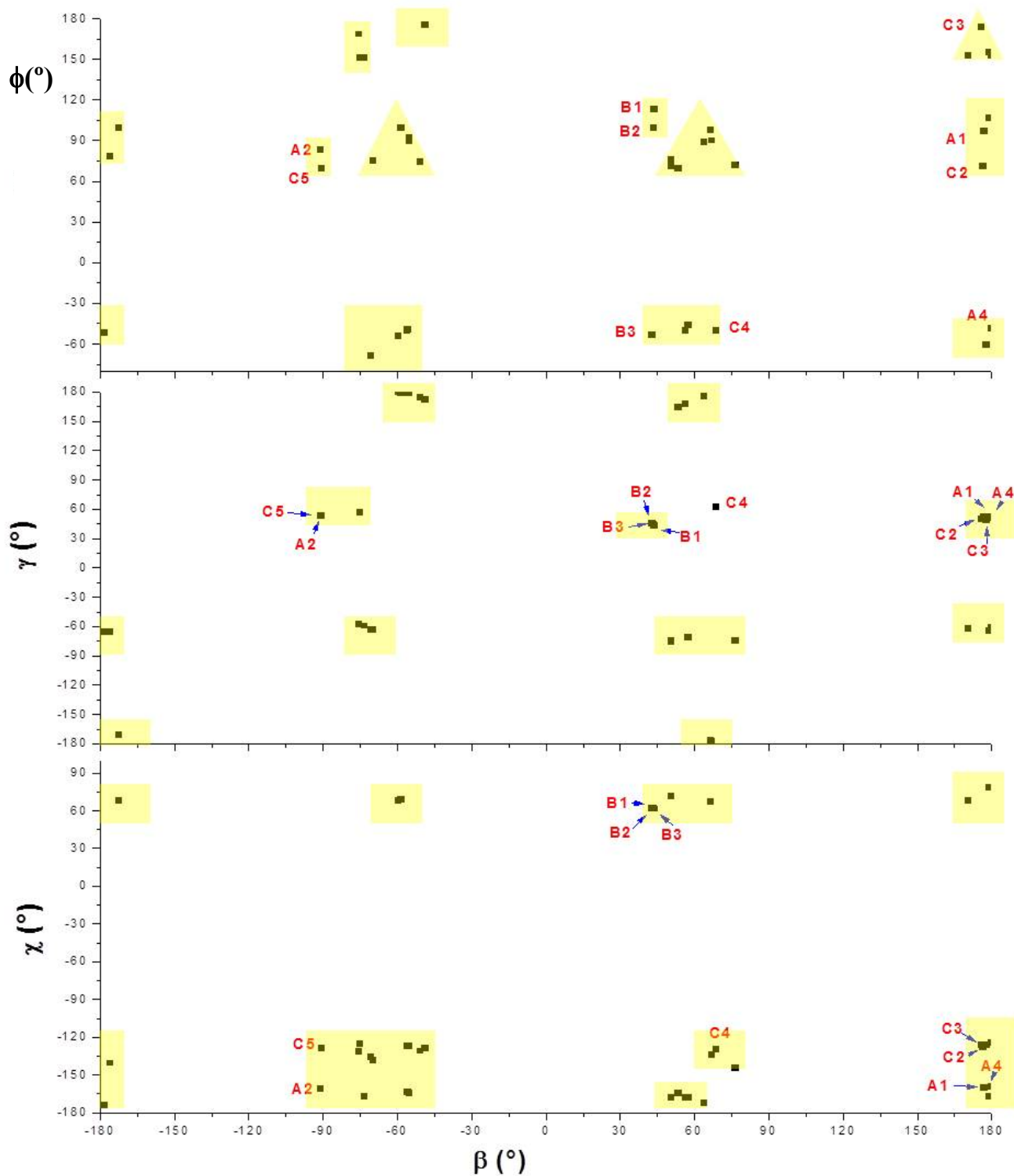
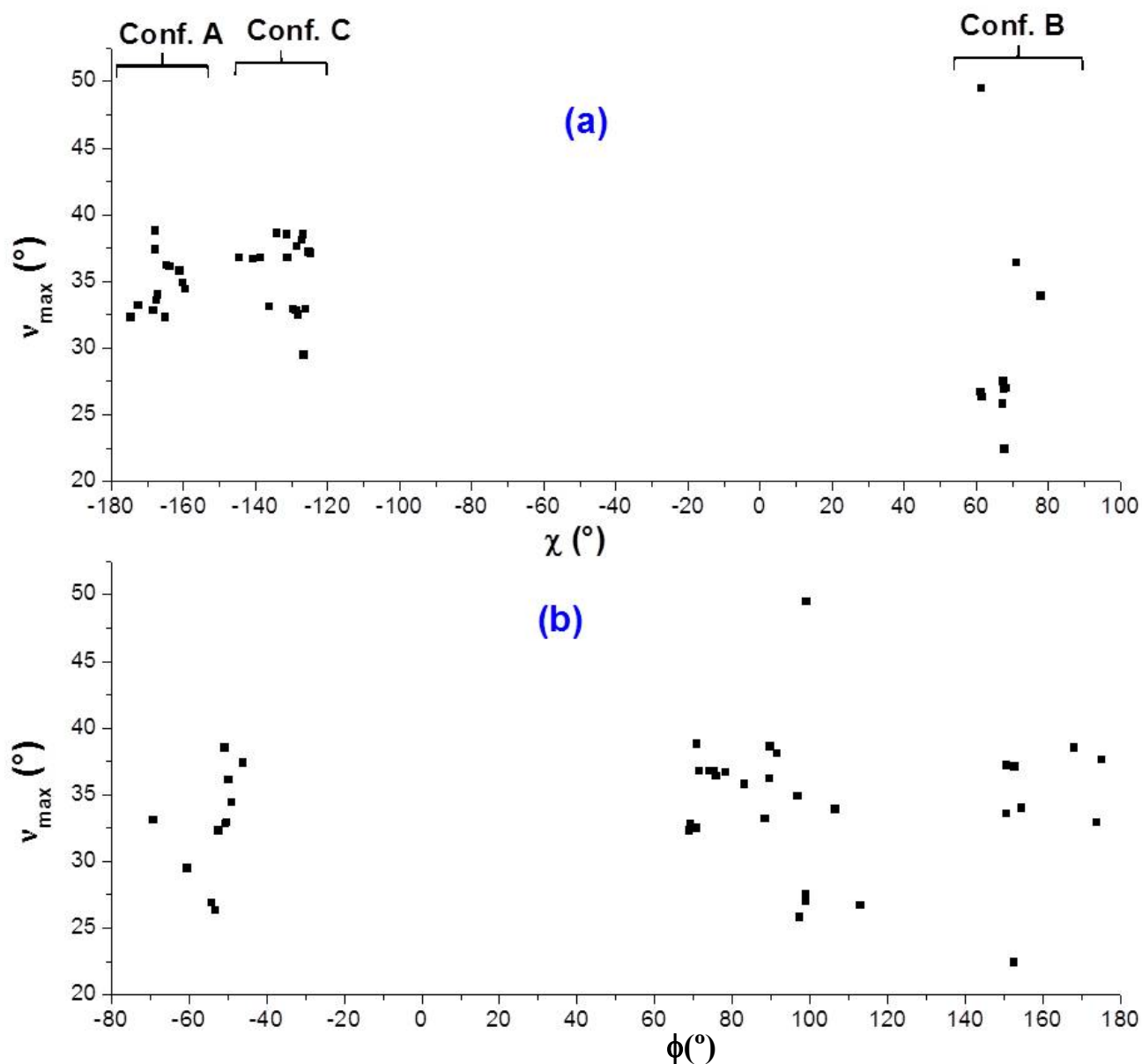


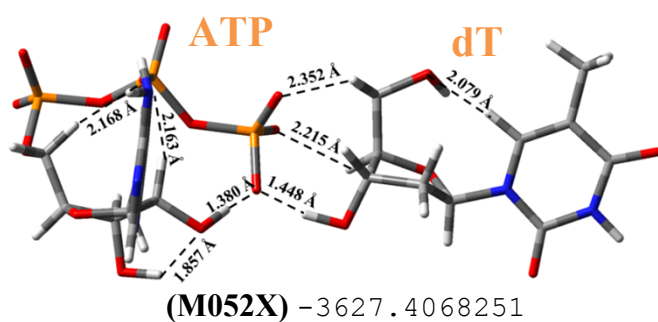
(Fig. 2-Sup). Relative energies of all the optimum stable conformers in AZT according to the values of the five exocyclic torsional angles: χ , β , γ , ϕ , and δ .



(Fig. 3-Sup). Distribution of all the optimum conformers according to the values of the exocyclic torsional angles ϕ , γ and χ versus β . 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 χ and ϕ versus v_{\max} .



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