

Supplementary Information

Does the tautomeric status of the adenine bases change under the dissociation of the $A^* \cdot A_{\text{syn}}$ Topal-Fresco DNA mismatch? A combined QM and QTAIM atomistic insight

Ol'ha O. Brovarets^{a,b,c}, Roman O. Zhurakivsky^{a,b} and Dmytro M. Hovorun^{a,b,c,✉}

^aDepartment of Molecular and Quantum Biophysics, Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine, 150 Akademika Zabolotnoho Str., 03680 Kyiv, Ukraine

^bResearch and Educational Center “State Key Laboratory of Molecular and Cell Biology”, 150 Akademika Zabolotnoho Str., 03680 Kyiv, Ukraine

^cDepartment of Molecular Biology, Biotechnology and Biophysics, Institute of High Technologies, Taras Shevchenko National University of Kyiv, 2-h Akademika Hlushkova Ave., 03022 Kyiv, Ukraine

✉Corresponding author. Email: dhovorun@imbg.org.ua.

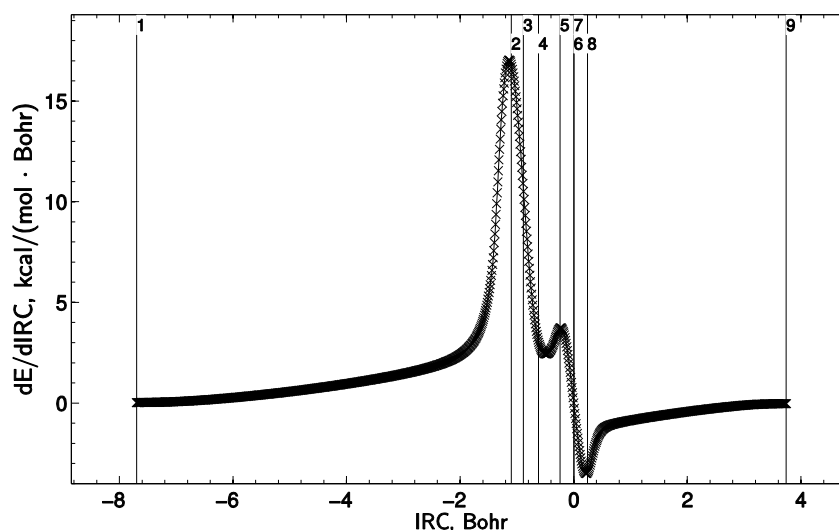


Fig. S1 Profile of the first derivative of the electronic energy E with respect to the IRC - $dE/dIRC$ - along the IRC of the $A^* \cdot A_{\text{syn}} \leftrightarrow A \cdot A^*_{\text{syn}}$ tautomerisation *via* the DPT obtained at the B3LYP/6-311++G(d,p) level of theory *in vacuo*.

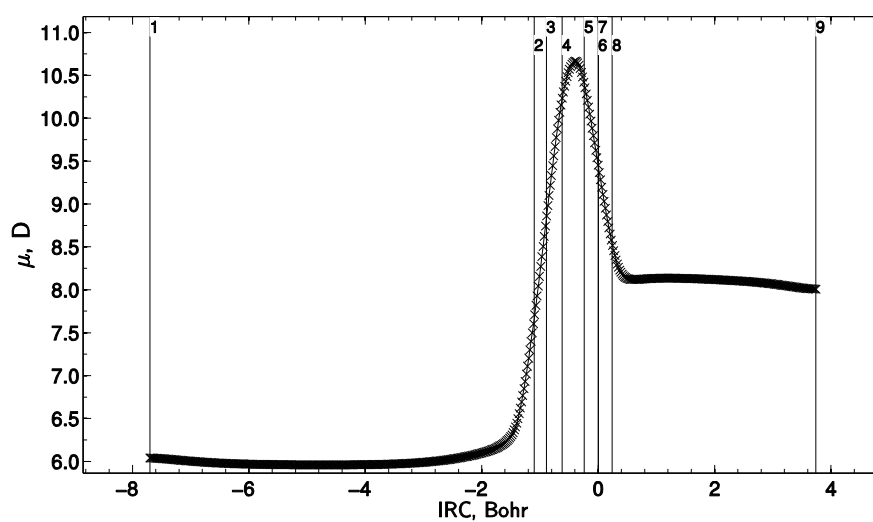


Fig. S2 Profile of the dipole moment μ of the base mispair along the IRC of the $A^* \cdot A_{\text{syn}} \leftrightarrow A \cdot A^*_{\text{syn}}$ tautomerisation *via* the DPT obtained at the B3LYP/6-311++G(d,p) level of theory *in vacuo*.