Supporting Information

Conformational Stabilities of Iminoallantoin and its Base Pairs in DNA: Implications for Mutagenicity

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Fig. S1: Structures of different tautomers of Ia1 in the R-stereoisomeric conformation (Ia1-R). The relative ZPE-corrected total energies (kcal/mol) calculated with respect to (a) by employing B3LYP/6-31+G* level of theory are shown in parentheses. The energies shown in brackets correspond to the equivalent tautomers of Ia1 in the S-stereoisomeric conformation (Ia1-S).
Fig. S2: Structures of different tautomers of Ia2 in the R-stereoisomeric conformation (Ia2-R). The relative ZPE-corrected total energies (kcal/mol) calculated with respect to (a) by employing B3LYP/6-31+G* level of theory are shown in parentheses. The energies shown in brackets correspond to the equivalent tautomers of Ia2 in the S-stereoisomeric conformation (Ia2-S).
Fig. S3: Structures of different tautomers of Ia3 in the R-stereoisomeric conformation (Ia3-R). The relative ZPE-corrected total energies (kcal/mol) calculated with respect to (a) by employing B3LYP/6-31+G* level of theory are shown in parentheses. The energies shown in brackets correspond to the equivalent tautomers of Ia3 in the S-stereoisomeric conformation (Ia3-S).
Fig. S4: Optimized structures of different rotamers of the most stable tautomer of 2'-deoxyIa in the R- and S-diastereoisomeric conformations in aqueous medium. The $\chi$ values of these rotamers obtained at the B3LYP and B3LYP-D3 (in bold) methods are shown for comparison. As the $\chi$ values are just higher than the permissible value of a $\text{syn}$-conformation in DNA ($\chi = 0$ to 90 deg), $N$-glycosidic bond rotation from $\text{anti}$-Ia to $\text{syn}$-Ia would be easy in DNA.
Table S1: The ZPE-corrected binding energies of different complexes involving the R-stereoisomer of Ia (Ia-R) in the *anti*- and *syn*-conformations as obtained in aqueous medium by employing different level of theories. The binding energies of T:G, G:C and T:A complexes are shown in parentheses for comparison. The absence of entry shows that the corresponding complex does not exist.

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*a*Obtained by single-point energy calculations by employing B3LYP/6-31+G* geometry.
Fig. S5: Different optimized structures of Ia-R:G complexes as obtained in aqueous medium by employing B3LYP/6-31+G* level of theory. In (c), (e), and (g) G binds with anti-Ia-R in the inverted orientation (G_{inv}). We noted that these complexes can also be formed by binding of G with the inverted anti-Ia-R (anti-Ia-R_{inv}).
Fig. S6: Different optimized structures of Ia-R:C complexes as obtained in aqueous medium by employing B3LYP/6-31+G* level of theory. In (f) C binds with $syn$-Ia-R in the inverted orientation ($C_{inv}$). We noted that this complex can also be formed by binding of C with the inverted $syn$-Ia-R ($syn$-Ia-$R_{inv}$).
Fig. S7: Different optimized structures of Ia-R:A complexes as obtained in aqueous medium by employing B3LYP/6-31+G* level of theory. In (b) and (i), A binds with anti-Ia-R and syn-Ia-R in the inverted orientation (A_{inv}) respectively. We noted that these complexes can also be formed by binding of A with the inverted Ia-R in the anti-(anti-Ia-R_{inv}) and syn-(syn-Ia-R_{inv}) conformations respectively.
Fig. S8: Different optimized structures of Ia-R:T complexes as obtained in aqueous medium by employing B3LYP/6-31+G* level of theory. In (b) and (i) T binds with anti-Ia-R and syn-Ia-R in the inverted orientation (T_{inv}) respectively. We noted that these complexes can also be formed by binding of T with the inverted Ia-R in the anti- (anti-Ia-R_{inv}) and syn- (syn-Ia-R_{inv}) conformations respectively.
Table S2: The XYZ-coordinates of the anti-La3\textsubscript{inv}-R:G complex

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Table S3: The XYZ-coordinates of the *anti*-Ia3-R:G complex

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Table S4: The XYZ-coordinates of the \textit{syn}-Ia3-R:G complex

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Table S5: The ZPE-corrected binding energies of different complexes involving the S-stereoisomer of Ia (Ia-S) in the anti- and syn-conformations as obtained in aqueous medium. The absence of entry shows that the corresponding complex does not exist.

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*Obtained by single-point energy calculations by employing B3LYP/6-31+G* geometry.
Fig. S9: Different optimized structures of Ia-S:G complexes as obtained in aqueous medium by employing B3LYP/6-31+G* level of theory. In (c), (e), and (g) G binds with anti-Ia-S in the inverted orientation (G_{inv}). We noted that these complexes can also be formed by binding of G with the inverted anti-Ia-S (anti-Ia-S_{inv}).
Fig. S10: Different optimized structures of Ia-S:C complexes as obtained in aqueous medium by employing B3LYP/6-31+G* level of theory. In (g), C binds with syn-Ia in the inverted orientation (C_{inv}). We noted that this complex can also be formed by binding of C with the inverted syn-Ia-S (syn-Ia-S_{inv}).
Fig. S11: Different optimized structures of Ia-S:A complexes as obtained in aqueous medium by employing B3LYP/6-31+G* level of theory. In (b) and (h), A binds with *anti*-Ia-S and *syn*-Ia-S in the inverted orientation (A$_{inv}$) respectively. We noted that these complexes can also be formed by binding of A with the inverted Ia-S in the *anti*-(anti-Ia-S$_{inv}$) and *syn*-(syn-Ia-S$_{inv}$) conformations respectively.
Fig. S12: Different optimized structures of Ia-S:T complexes as obtained in the aqueous medium by employing B3LYP/6-31+G* level of theory. In (b) and (i) T binds with *anti*-Ia-S and *syn*-Ia-S in the inverted orientation (T$_{inv}$) respectively. We noted that these complexes can also be formed by binding of T with the inverted Ia-S in the *anti-* (*anti*-Ia-S$_{inv}$) and *syn-* (*syn*-Ia-S$_{inv}$) conformations respectively.