

Theoretical Description of the Coding Potential of Diamino-5-formamidopyrimidines*

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The results of geometry optimisation of possible Watson-Crick-like pairs of 2,6-diamino-4-oxy-5-formamidopyrimidine (fapy-adenine) or 4,6-diamino-5-formamidopyrimidine (fapy-guanine) were presented. In the absence of the external field the fapy-adenine is able to form pairs with all four canonical nucleic acid bases. However, pairs with guanine, cytosine and thymine the most stable are. Thus, the potential miscoding abilities may be observed. In contrast, in the presence of the external field the mispairing abilities of fapy-adenine become insignificant since the most stable dimers are formed with thymine.

The pairing properties of fapy-guanine are complex and depend on its tautomeric form. In the absence of an external field the 4-enol-6-keto-diamino tautomer of fapyG is able to form stable dimers with thymine and cytosine, while the 4,6-diketo-diamino tautomer forms the most stable pairs with cytosine and guanine. The presence of the water solvent does not significantly alter the pairing abilities of fapy-guanine. However, pairs with thymine are at least as stable as the Watson-Crick GC pair. Thus, in polar conditions the mispairing potential of fapyG will be extended and may be enriched by potential GC \rightarrow AT transition.

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