

Mechanism underlying the nucleobase-distinguishing ability of benzopyridopyrimidine (BPP).

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Streszczenie

Benzopyridopyrimidine (BPP) is a fluorescent nucleobase analogue capable of forming base pairs with adenine (A) and guanine (G) at different sites. When incorporated into oligodeoxynucleotides, it is capable of differentiating between the two purine nucleobases by virtue of the fact that its fluorescence is largely quenched when it is base-paired to guanine, whereas base-pairing to adenine causes only a slight reduction of the fluorescence quantum yield. In the present article, the photophysics of BPP is investigated through computer simulations. BPP is found to be a good charge acceptor, as demonstrated by its positive and appreciably large electron affinity. The selective quenching process is attributed to charge transfer (CT) from the purine nucleobase, which is predicted to be efficient in the BPP-G base pair, but essentially inoperative in the BPP-A base pair. The CT process owes its high selectivity to a combination of two factors: the ionization potential of guanine is lower than that of adenine, and less obviously, the site occupied by guanine enables a greater stabilization of the CT state through electrostatic interactions than the one occupied by adenine. The case of BPP illustrates that molecular recognition via hydrogen bonding can enhance the selectivity of photoinduced CT processes.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>