

Base pairs and their higher order structures

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Nucleobases form base pairs, and the question of what the main driving forces behind the base pair formation are is a prevalent one. In our approach to tackle this question we used data from Cambridge Structural Database – we searched for base pair types found in small molecule crystal structures. Obtained base pair types, their frequencies of occurrence and protonation patterns lets us analyze the tendencies of nucleobases to form base pairs.

The reason of why such tendencies occurred varied by the nucleobase, but some general trends were present. The protonation patterns followed the pK_a values of particular nucleobases and the hydrogen bond lengths did not depend on the charge of nucleobases. We compared our findings with analogous data stored in the RNA Basepair Catalog – we found base pairs exclusive for small molecule crystal structures, exclusive for RNA crystal structures and these which were present in both environments. Basing on the frequencies of base pairs, we proven that the pairs often occurring in crystals of small molecules also often occur in RNA crystals [1].

Many base pairs can form higher order structures (Fig. 1) – either some larger aggregates, ribbons, tetramers or whole layers. We wanted to see if there are any rules that govern over the tendency to form particular higher order structure. Is it more of a question of strength of hydrogen bonds (when hydrogen bonds incorporating O or N atoms are favored over these with C), overall interaction energy, or is it rather determined by a simple geometry?

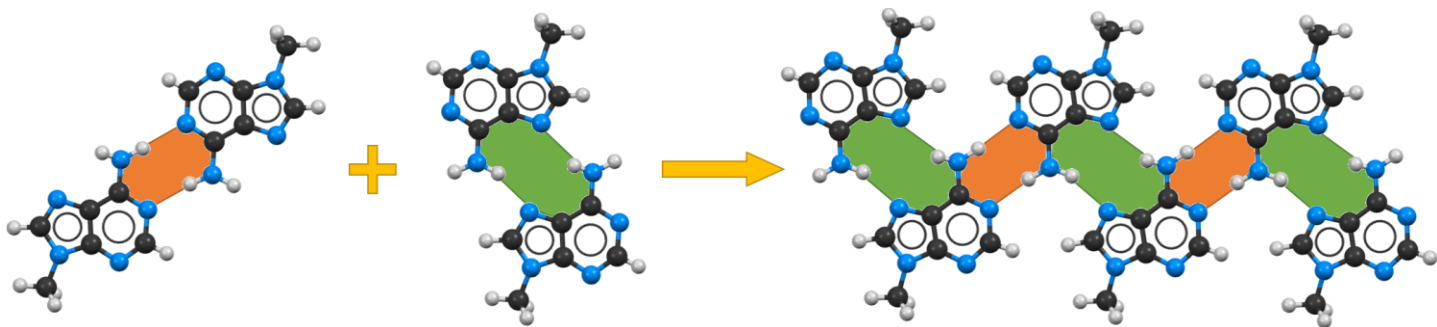


Figure 1. Formation of higher order structures from base pairs.

[1] Cabaj, M. K., Dominiak, P. M. (2020). *NAR*, **48**, 8302.

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