

5-Substituted uracils: Another brick in the quad

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5-Substituted uracils (5sUs) are considered theoretically and experimentally as new building blocks in quadruplex structures. DFT calculations performed a-prior to experimental investigations and predicted the formation of 5sUs based tetrameric structures. Central cation binding as well as the stacking capacity of layers were examined similar to previous studies [1-3]. The stacking energy is very close to the interaction of two xanthine (Xa) layers, and 5sU tetrad cover almost exactly the same area as Xa or guanine tetrads. This latter property provides the possibility to combine Xa and guanine tetramers with 5sU based layer and form a common central channel within quadruplex structure.

Following the theoretical investigations, synthetic works has been started and the existence of 5sU complexes were pointed out by mass-spectrometry. Both homo 5sU and mixed (5sU with Xa) systems were found, as well as structures with 2,3,4, ... and 8 units. We are convinced that the suggested molecules can be used as new building blocks in many different applications including aptamers, bio-sensors or artificial ion channels.

References

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