5 Conclusions

In the ia) part of present work we compared the stability and molecular interaction between adenine...thymine, guanine...cytosine and their methylated analogues with a small number of water and organic solvent molecules (CH_3OH, DMSO, $CHCl_3$).

We observed completely different interactions between the bases and the solvents studied. Whereas water and CH_3OH can stabilize the S structures of the base pairs by a higher number of H-bonds than is possible in HB pairs, the $CHCl_3$ molecule lacks such a property, and the HB structures with molecule(s) of solvent situated above or below the base pair are preferred. The DMSO molecule is unique by its dimension in comparison with other solvents, and the T structures are the most abundant ones.

In the ib) part of present work based on the MD, SCC-DDFTB-D and COSMO calculations of modified nucleobases **X** incorporated to DNA duplex we made following conclusions:

i) Replacing nucleic acid base by modified nucleobase **X** leads mostly to structural changes of the central base pair (stack arrangement of central modified base pairs). Only with the smallest modified nucleobase **P** the central base pairs (A-**P**, **P**-T) stay planar. In the case of **B**-T, A-**B** or **D**-**D** in specific orientation, one of the modified nucleobase **X** was forced out from DNA duplex.

ii) Increasing aromaticity of modified nucleobase **X** increases the stacking stabilization.

iii) The highest selectivity among all base analogue studied was found for modified nucleobase **D**.

In the second part of present work, we used for the calculation of reduction potentials of derivatives of nucleobases linked with transition metals (Ru^{2+}, Os^{2+}) complexes the DFT and COSMO methods and compared our results with experimental values. We observed, that in the case of Ru^{2+} complexes the calculated reduction potentials of oxidation agreed quite well with experimental values, whereas in the case of Os^{2+} complexes, the quite strong disagreement was observed. This can be explained by the spin orbit coupling, which was neglected in our calculations and plays in the Os^{2+} complexes more significant role, than in Ru^{2+} complexes. The interpretation of calculated reduction potentials was more

complicated, but in general, the calculated data were in the range of experimental values.

The six original research papers that complement the thesis are enclosed in the Appendices.