

## CONCLUSIONS

- New strategy for ellipticine synthesis was proposed. The yields of the synthesis are very high and pure product is obtained. The strategy was verified with the synthesis of other ellipticine derivatives.
- Benzylic oxidations of ellipticine and 1,4-dimethylcarbazole were studied and 13-hydroxyellipticine was synthesised.
- Three empirical potentials were compared with reference *ab initio* data of ellipticine derivative – DNA base pair.
- The empirical potentials calculate interaction energies of the complexes quite well (especially the A-ff86 and the LH potentials) but they fail in the search of global energy minima geometries.
- Interactions of ellipticine and 9-hydroxyellipticine with two oligonucleotides were studied in two buffers (weakly acidic and neutral, ellipticine is protonated in the acidic buffer).

- Using two-dimensional NMR techniques assignment of all hydrogen signals of oligonucleotides CGCTAGCG and ATAGCTAT was done.
- The most important interaction of the ellipticine derivatives with the oligonucleotides is intercalation, but in the acidic buffer ellipticine can form also non-intercalative (bond to the minor or to the major groove) complexes with the oligonucleotides.
- Both ellipticine derivatives destabilised the duplex structure of the oligonucleotide ATAGCTAT in acidic environment.
- In the neutral buffer the life-time of ellipticine complexes with the oligonucleotide CGCTAGCG at 25 °C is approximately 7 ms, in acidic buffer is the life-time shorter.