

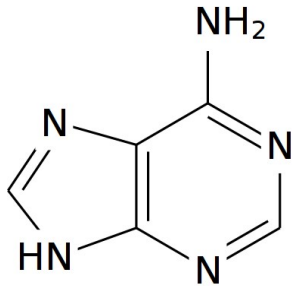
Bioinformatika III

Trimačių struktūrų analizė ir spėjimas

Paskaita 7 – nukleorūgščių molekulių
geometrija

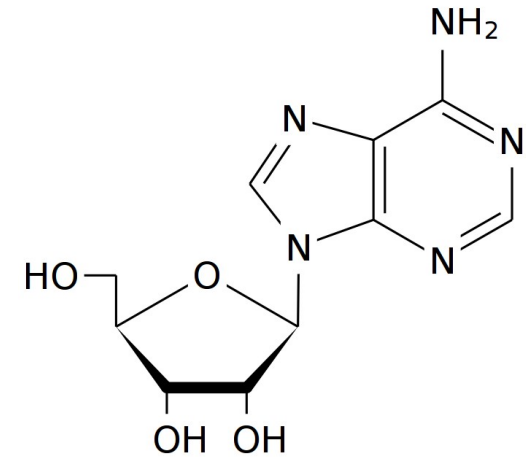
Saulius Gražulis
2011 m.

Nukleotidų cheminė struktūra

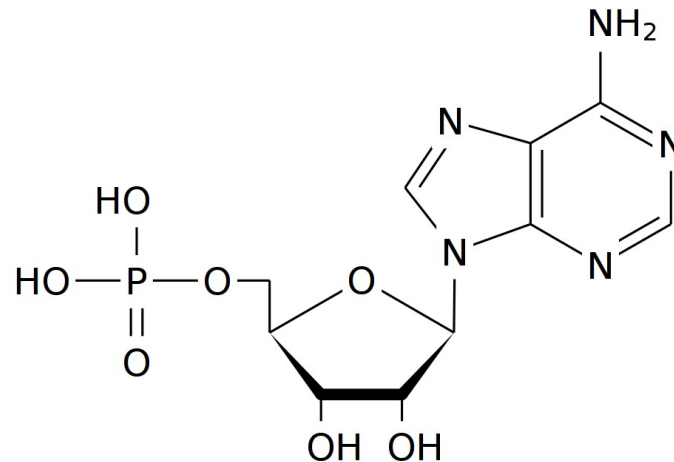


Bazės

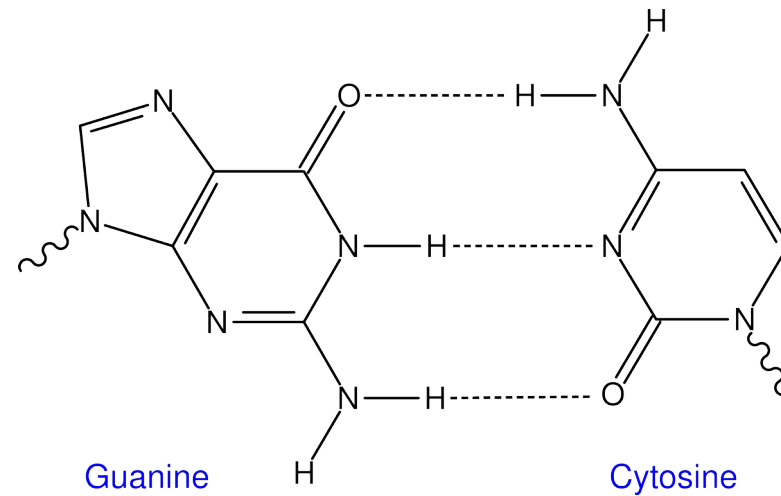
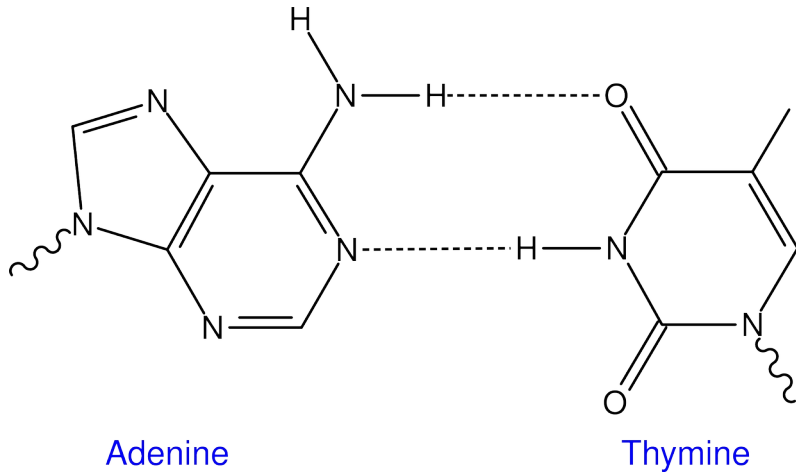
Nukleozidai
(glikozidai)



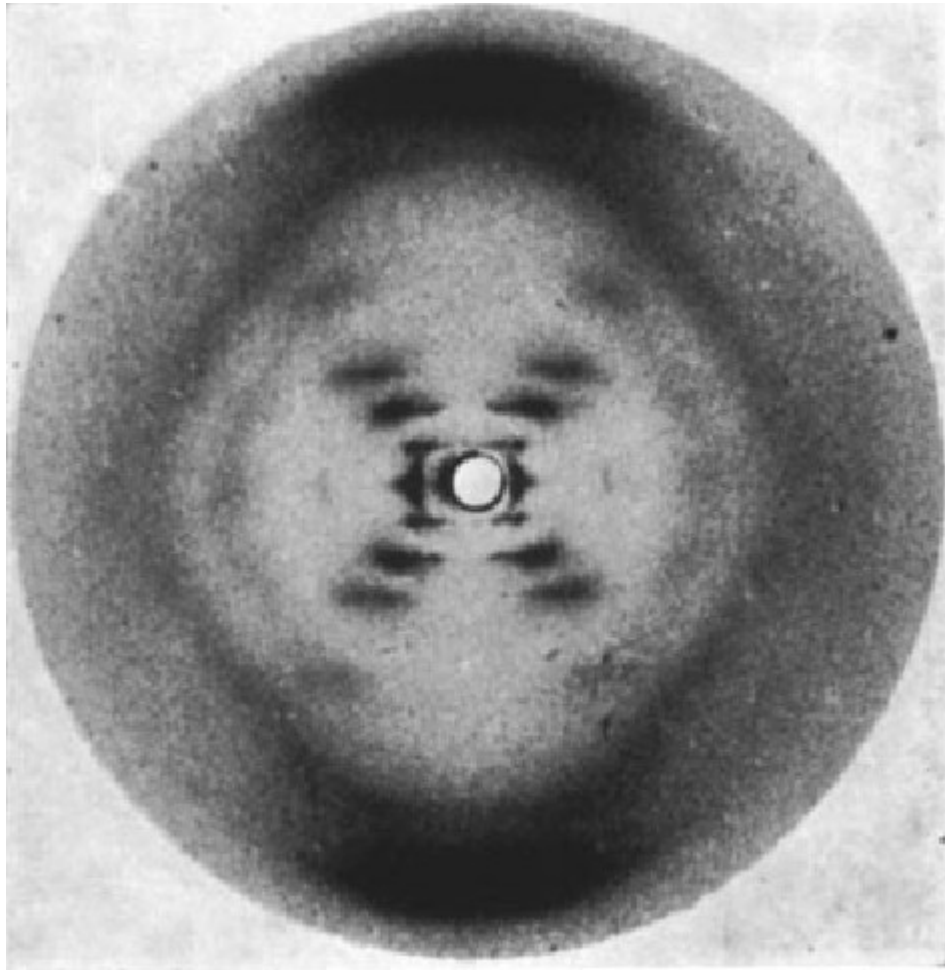
Nukleotidai
(glikozidfosfatai)



Vatsono-Kriko (Watson-Crick) poros



RA ir Watsono-Kriko modelis



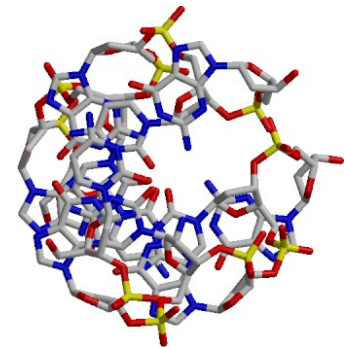
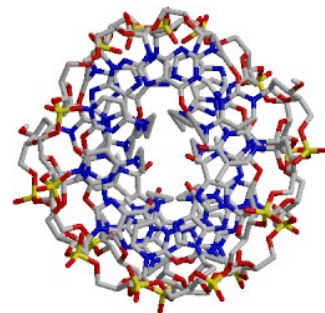
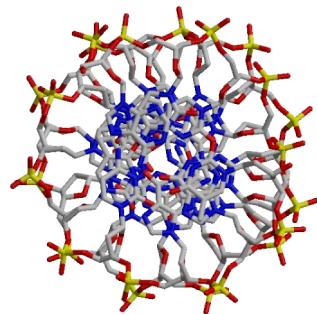
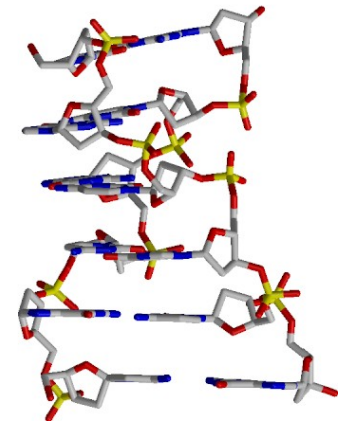
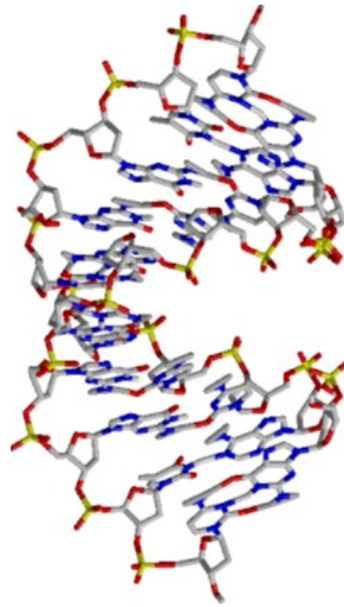
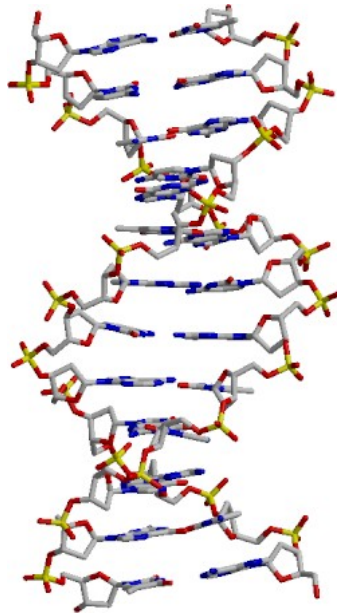
Franklin, R. E. & Gosling, R. G.
(1953) *Nature* **171**, 740



This figure is purely diagrammatic. The two ribbons symbolize the two phosphate—sugar chains, and the horizontal rods the pairs of bases holding the chains together. The vertical line marks the fibre axis

Watson & Crick, (1953) *Nature* **171**, 737

Dviguba spirale



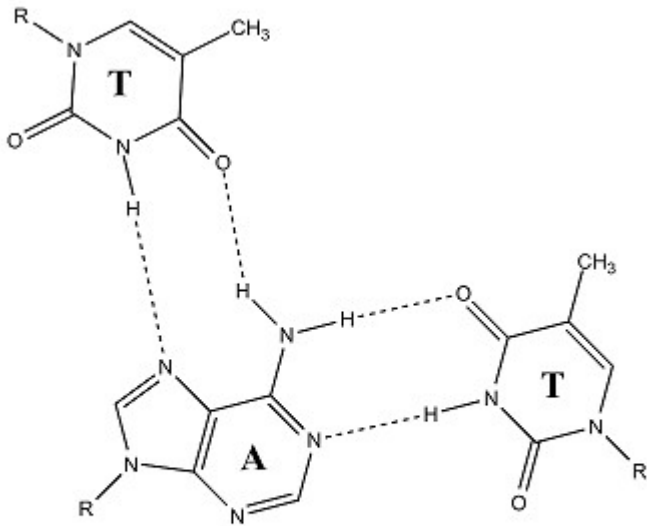
B forma (DNR)

A forma (DNR)

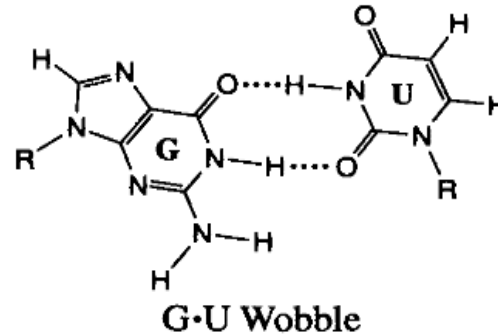
Z forma (DNR)

„Nestandartinės“ poros, tripletai, kvadrupleksai

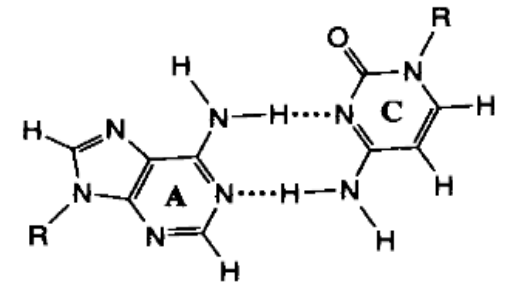
Hugstino bazių poros
(Hoogsteen base pair)



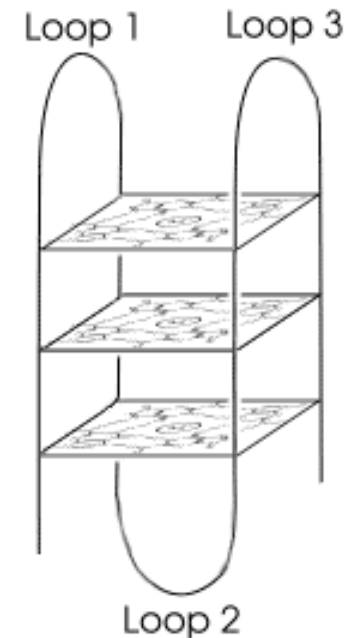
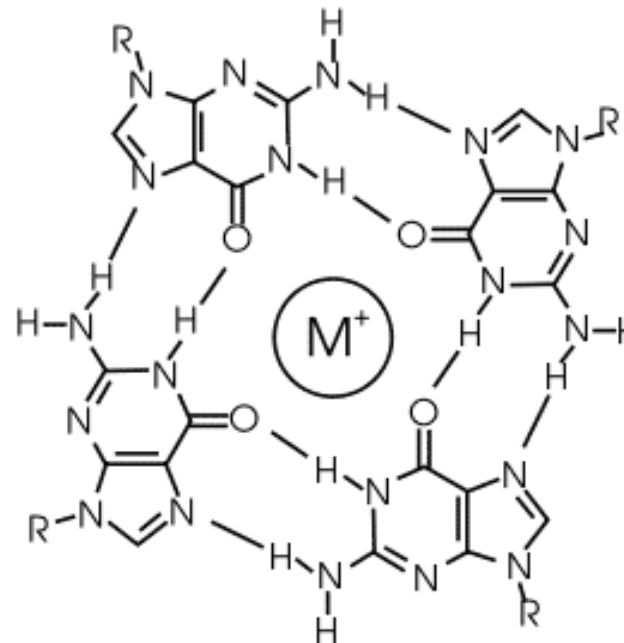
TA*T



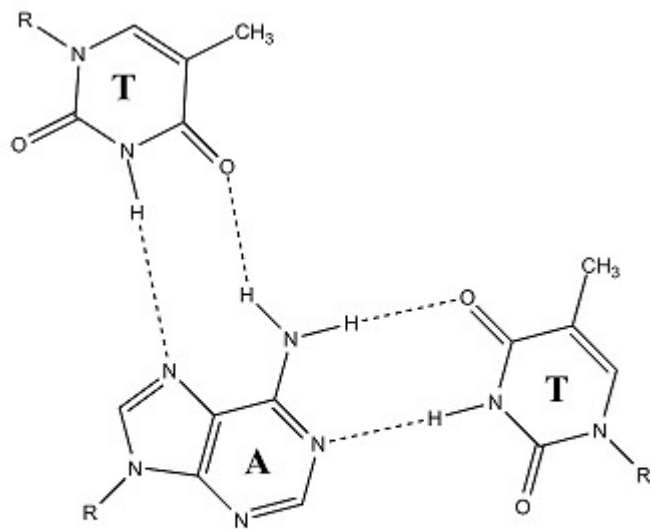
G•U Wobble



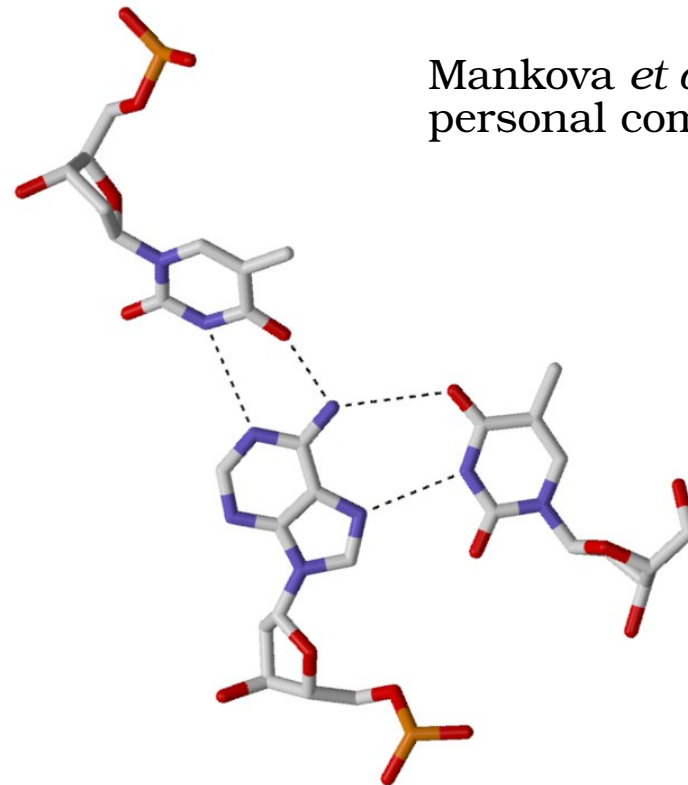
A•C Reverse wobble



Hugstino poros eksperimente



TA*T



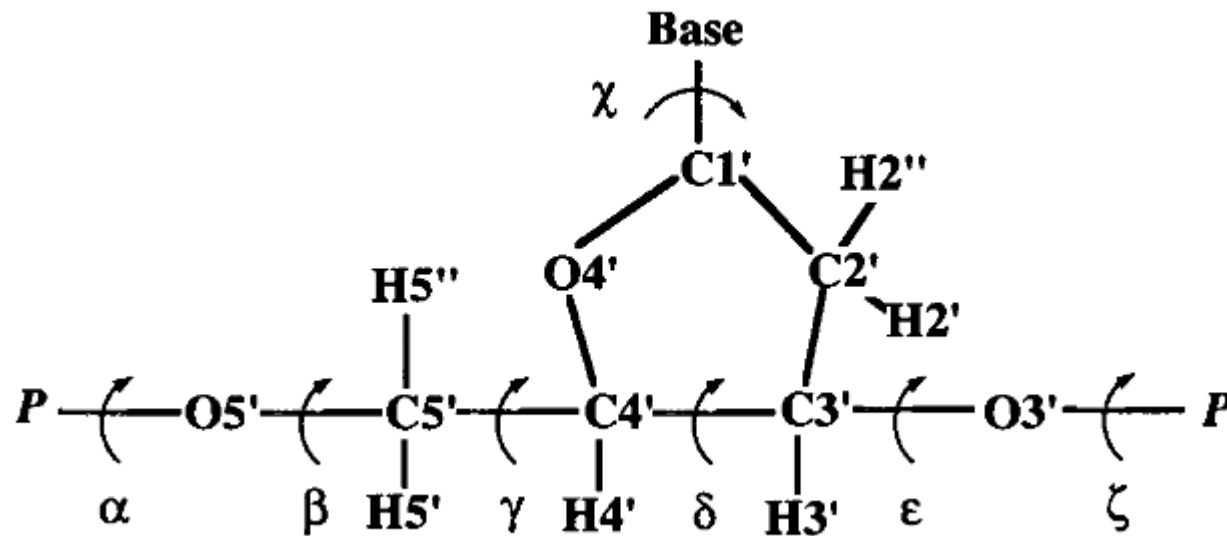
Mankova *et al.*,
personal comm.

Wikipedia:

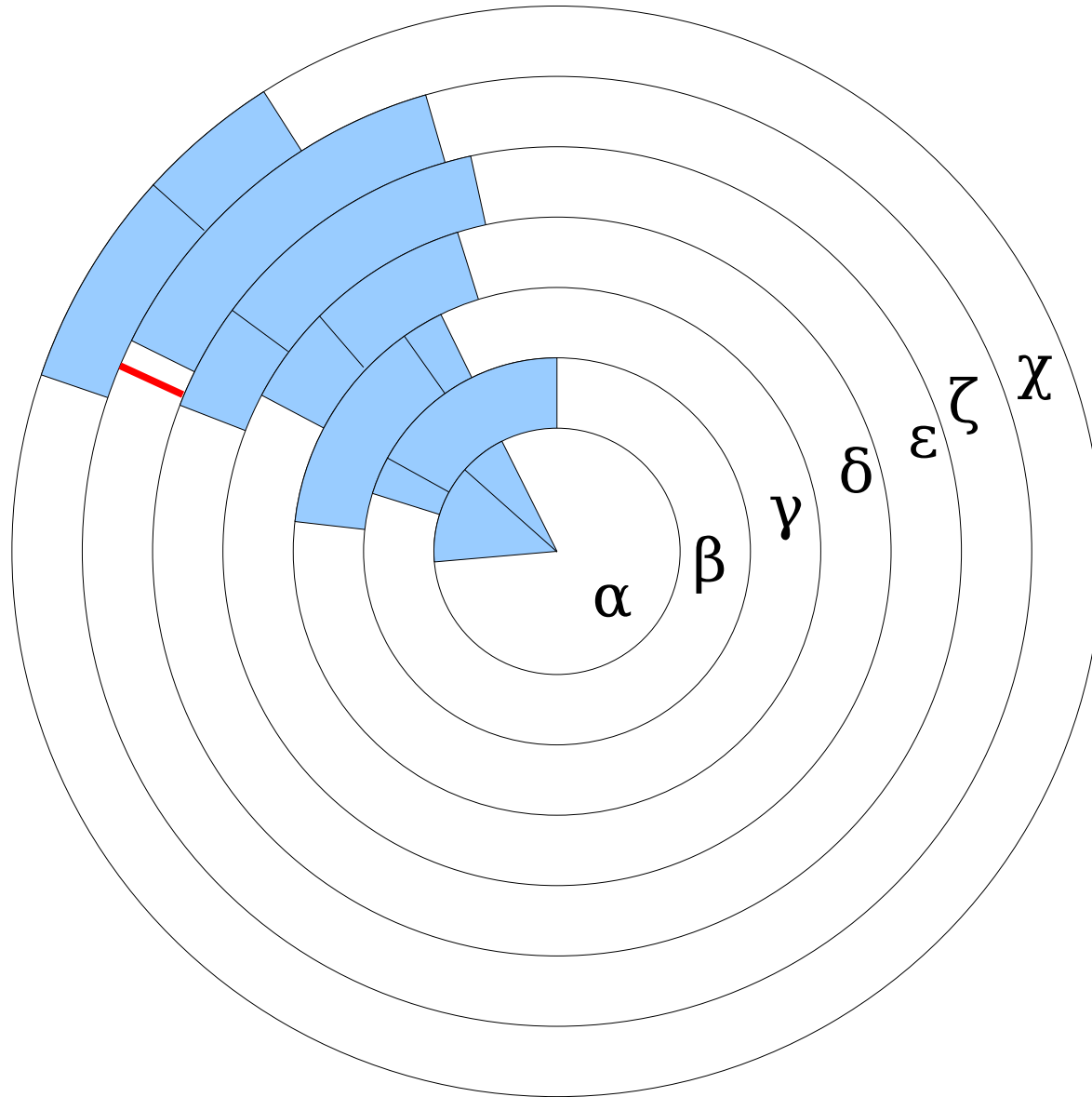
http://en.wikipedia.org/wiki/Hoogsteen_base_pair

<http://upload.wikimedia.org/wikipedia/commons/0/06/Hoogsteen.png>

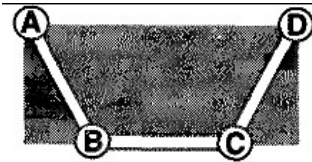
Nukleotidų jungčių kampai



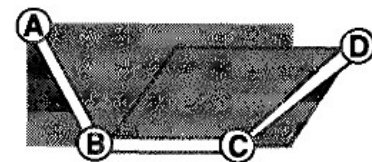
Valentinių kampų diagramos



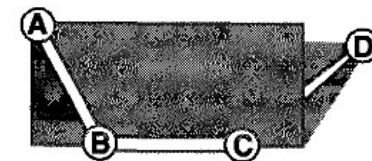
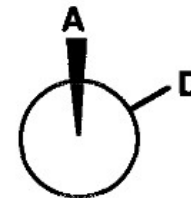
Valentinių kampų reikšmės



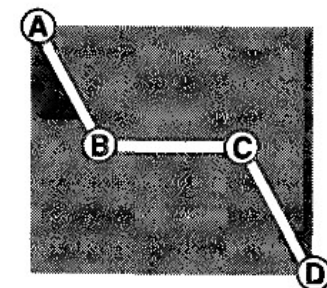
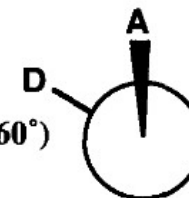
cis ($\theta = 0^\circ$)



gauche⁺ ($\theta = +60^\circ$)



gauche⁻ ($\theta = -60^\circ$)

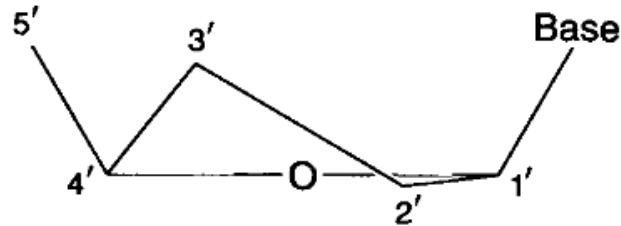


trans ($\theta = 180^\circ$)

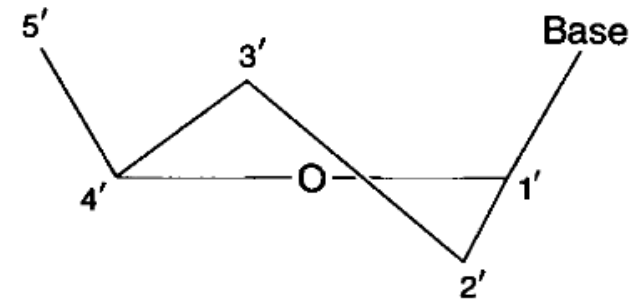


Cukraus žiedo konformacija

North (N) conformers—
A-form double strands

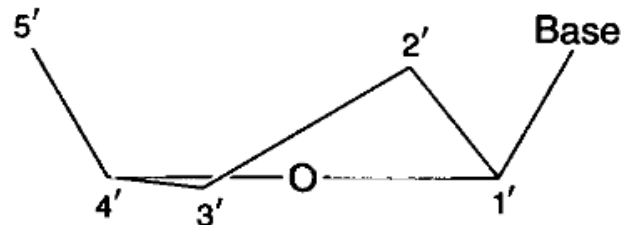


3'-endo
Phase angle, $P = 18^\circ$
Envelope

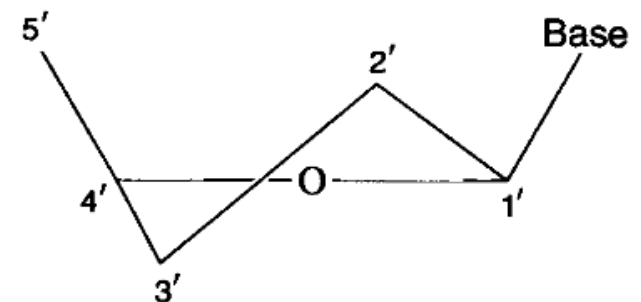


3'-endo, 2'-exo
Phase angle, $0^\circ < P < 18^\circ$
Twist

South (S) conformers—
B-form double strands

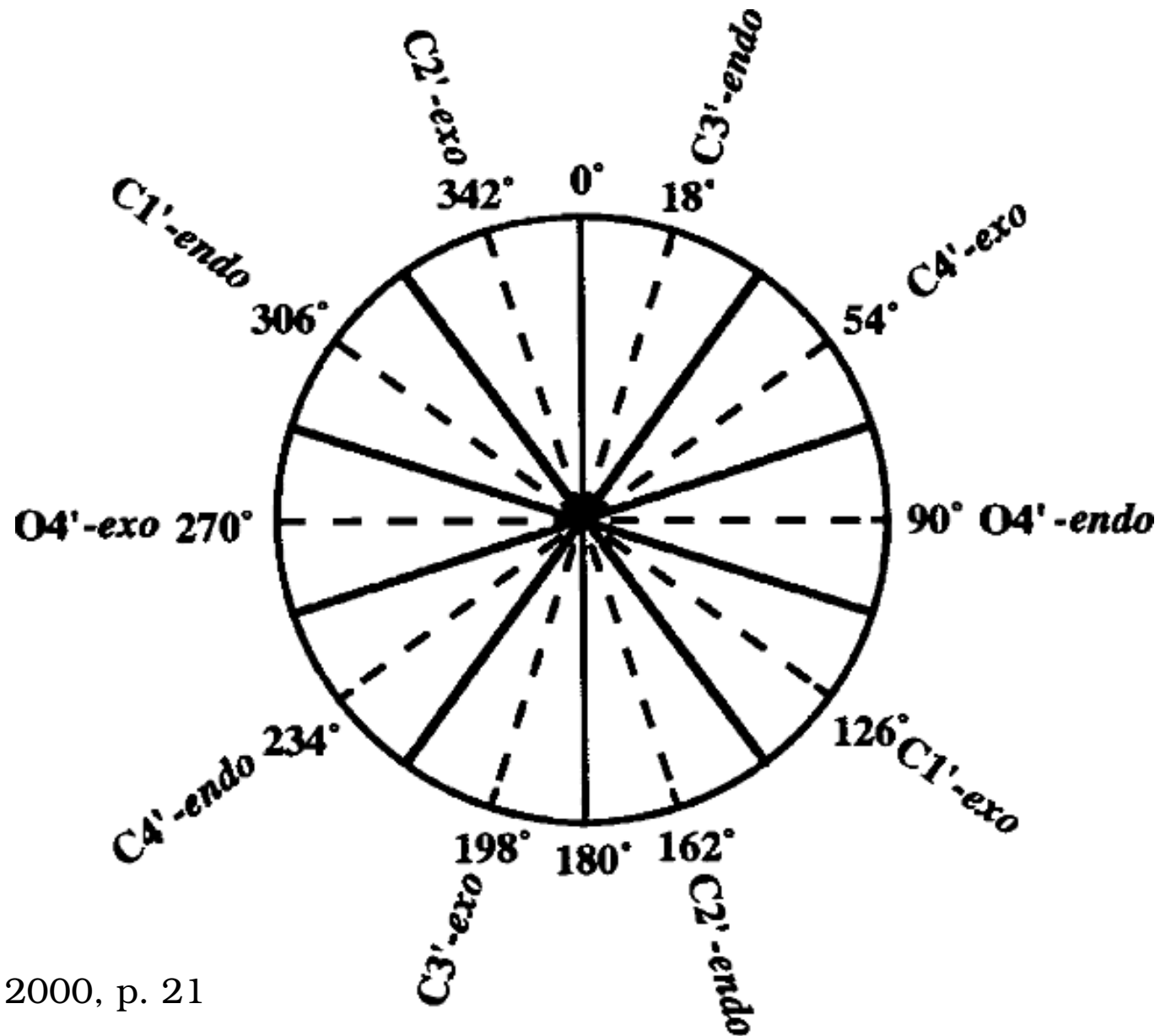


2'-endo
Phase angle, $P = 162^\circ$
Envelope

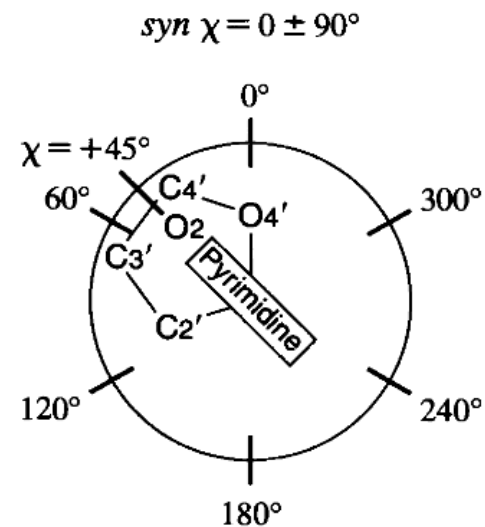
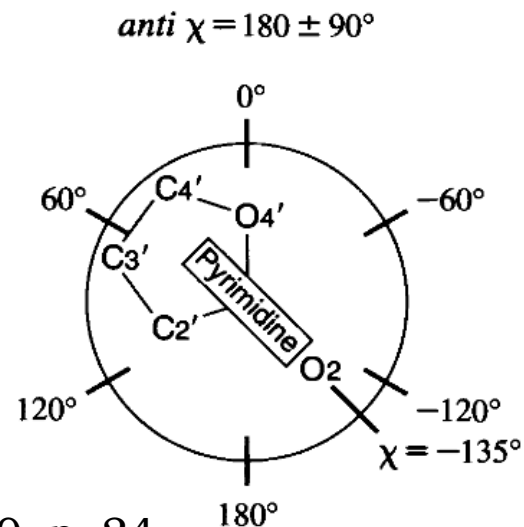
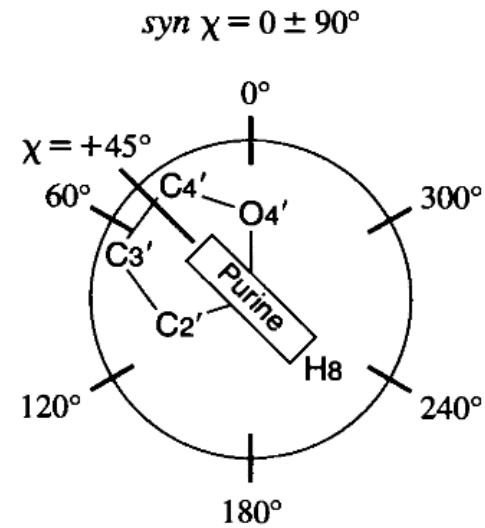
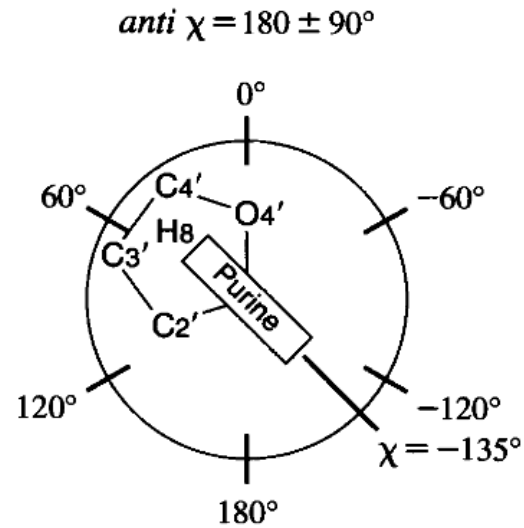


2'-endo, 3'-exo
Phase angle, $162^\circ < P < 180^\circ$
Twist

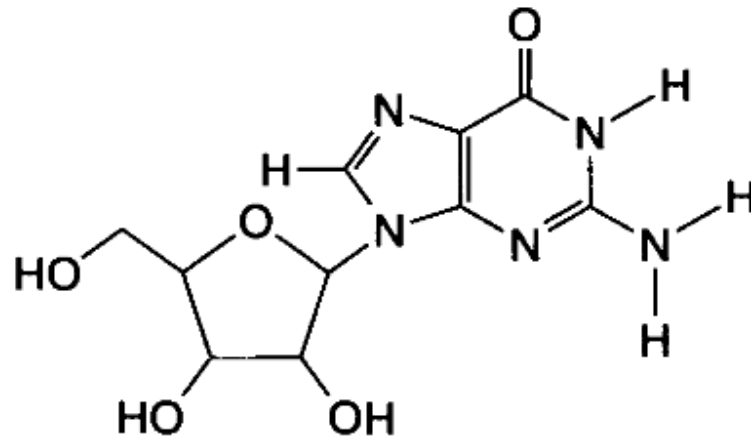
Pseudorotācijas kampai



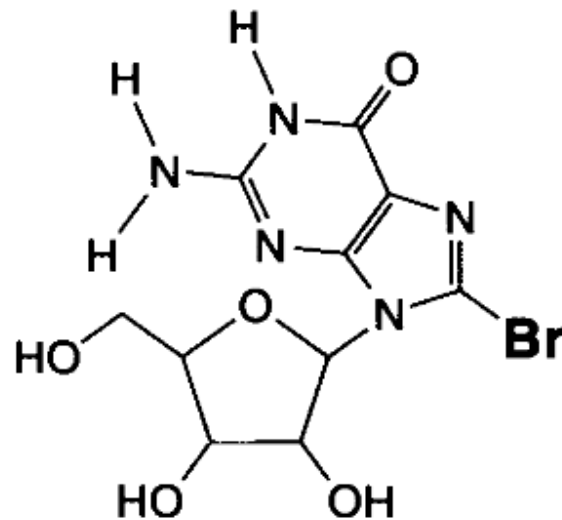
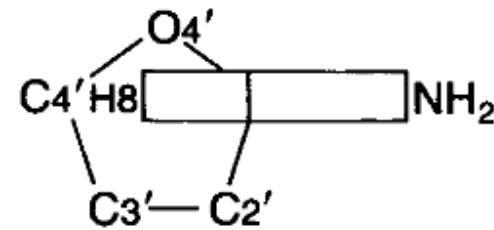
Syn ir *anti* konfigurācijas



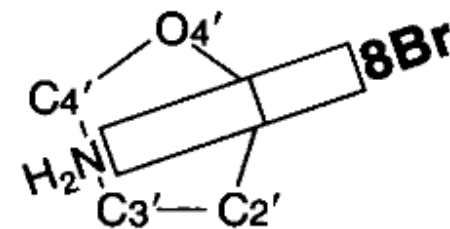
Didelio pakaito (Br) įtaka



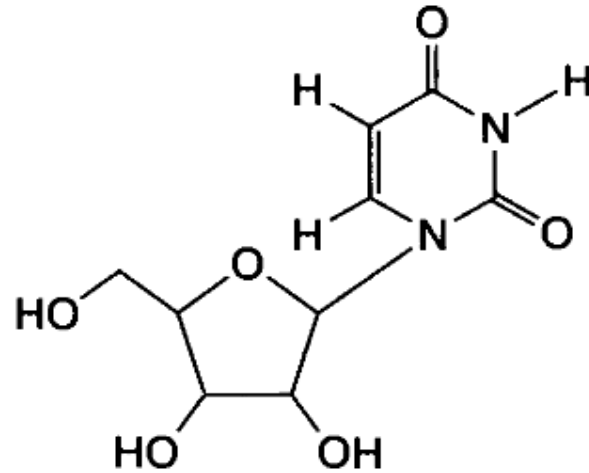
anti Guanosine



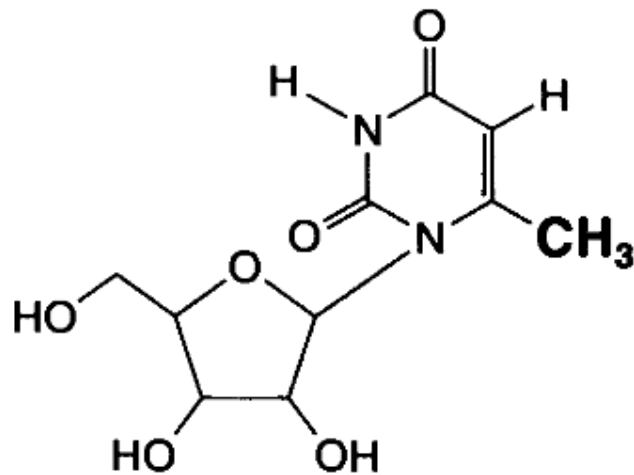
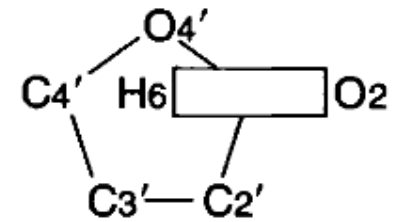
syn 8-Bromoguanosine



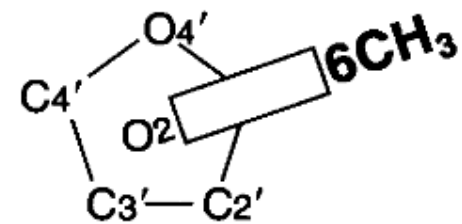
Syn/Anti variantai



anti Uridine



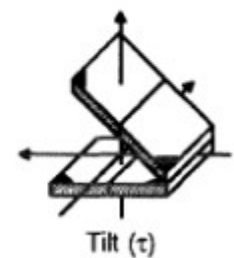
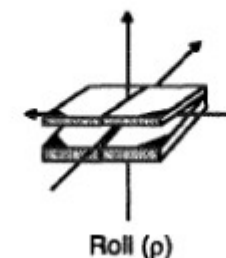
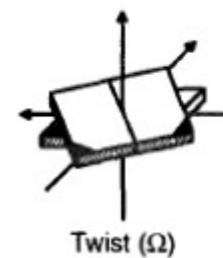
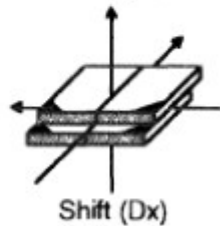
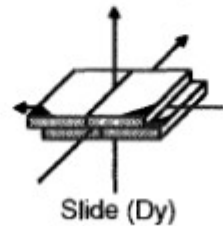
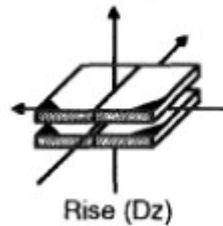
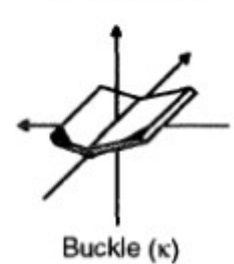
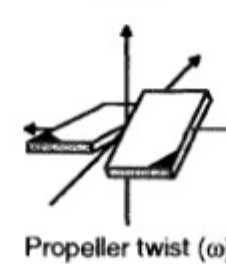
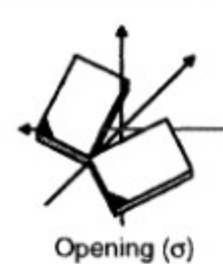
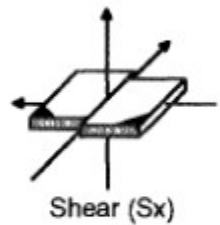
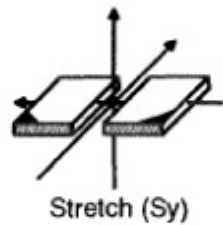
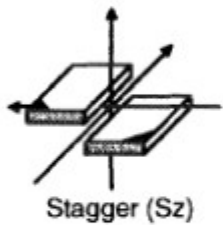
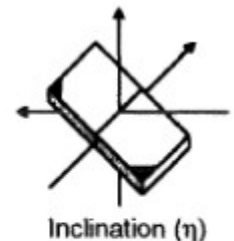
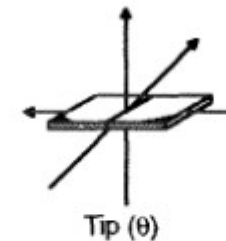
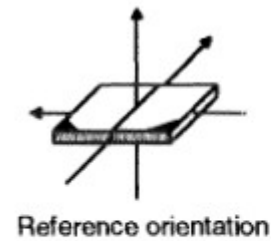
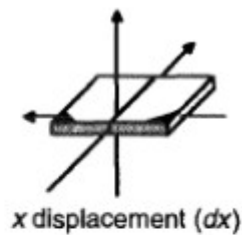
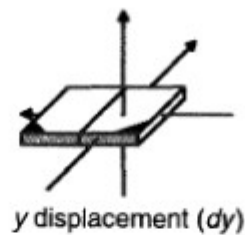
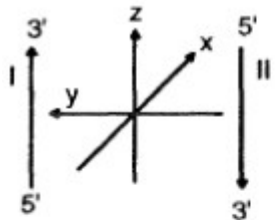
syn 6-Methyluridine



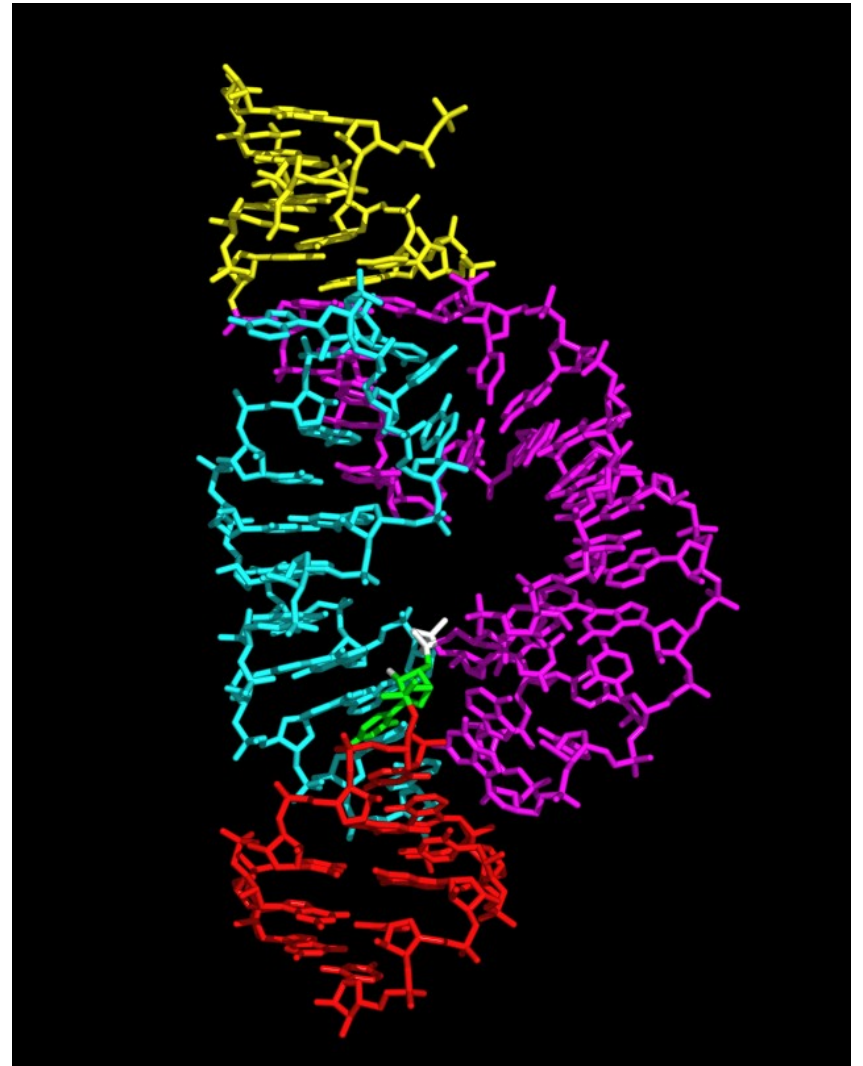
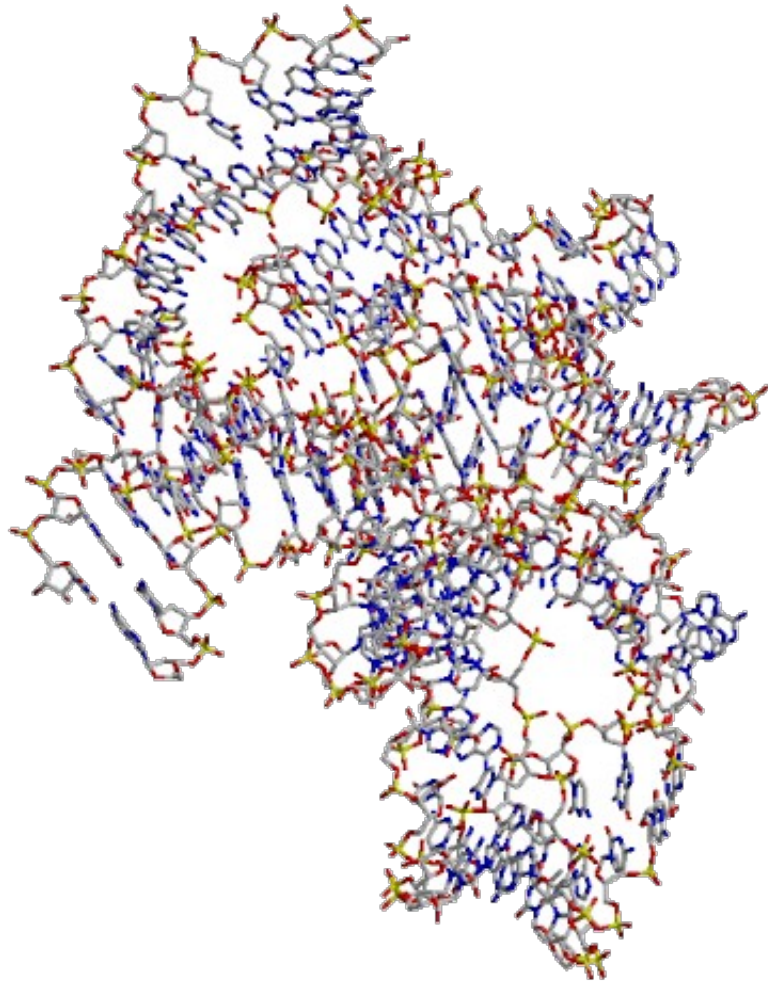
Bazių porų tarpusavio padėtis

Transliacija

Posūkis



RNR antrinēs struktūros

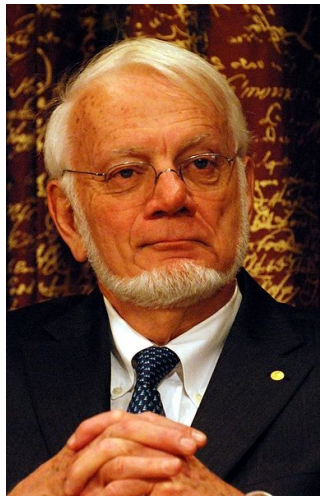


Hammerhead rybosime

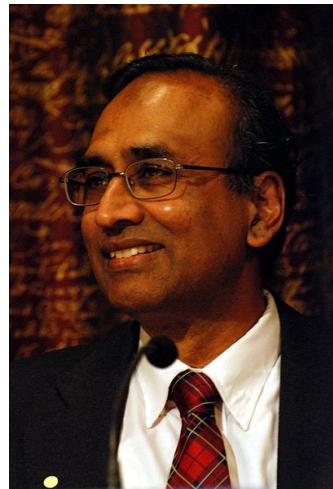
Ribosoma



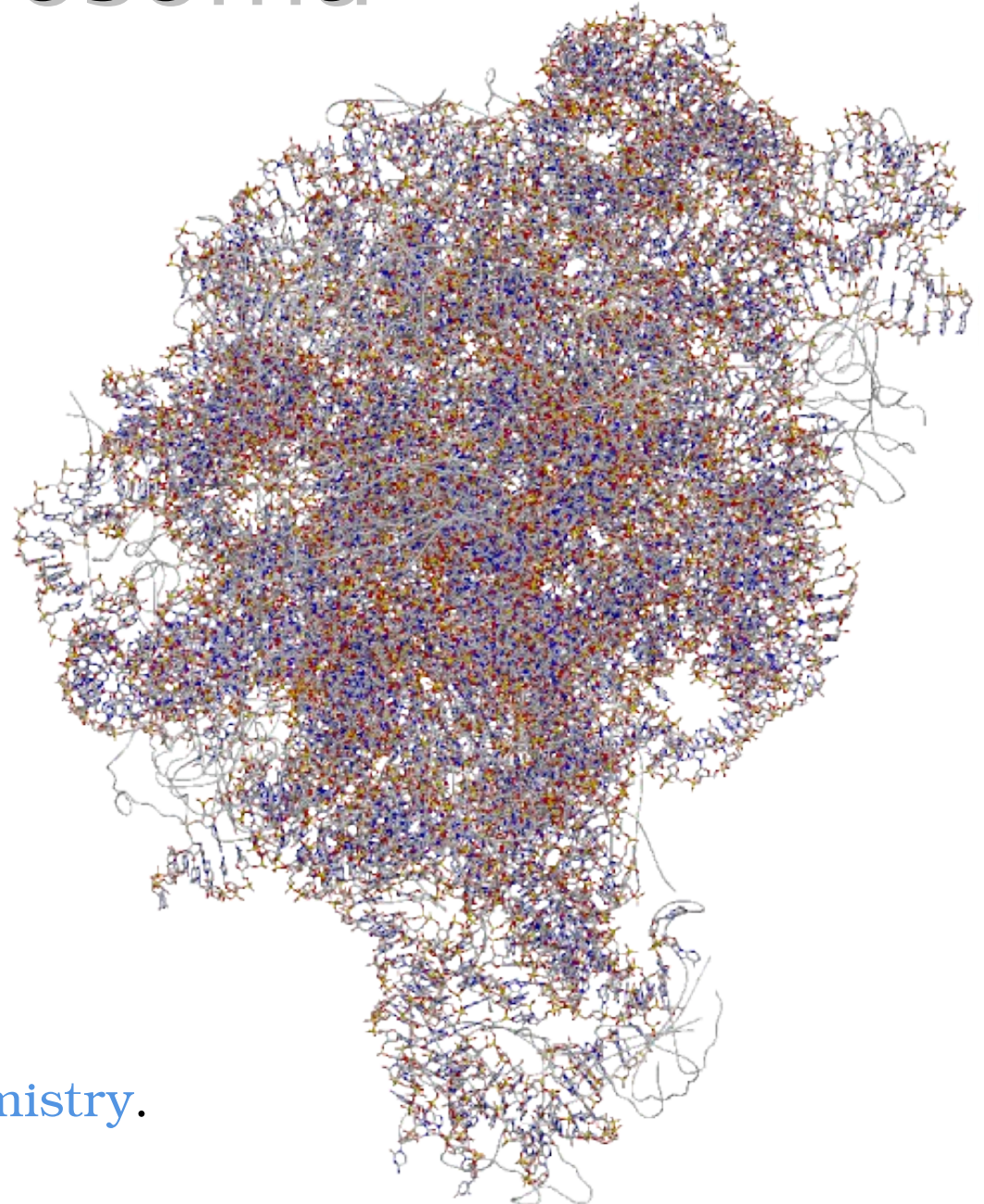
Ada Yonath



Thomas A. Steitz



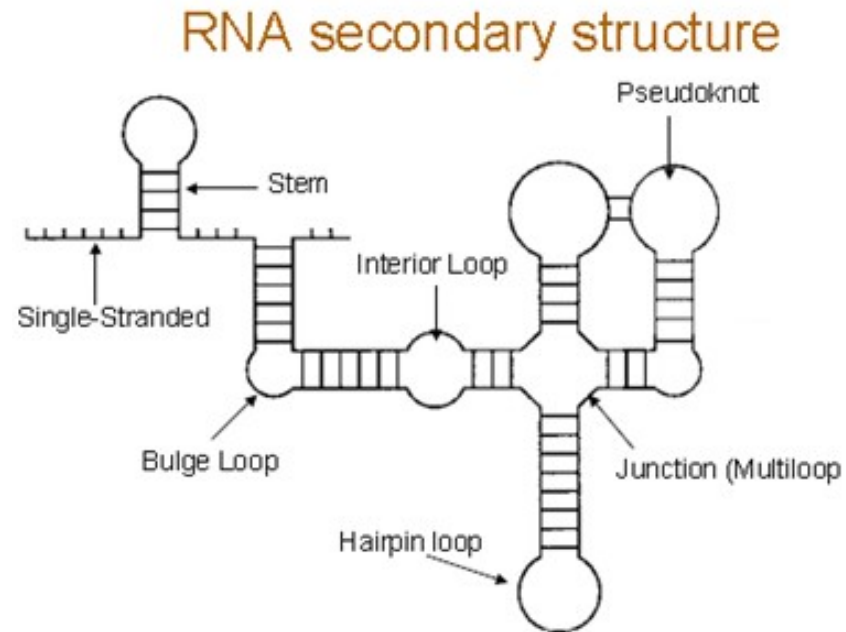
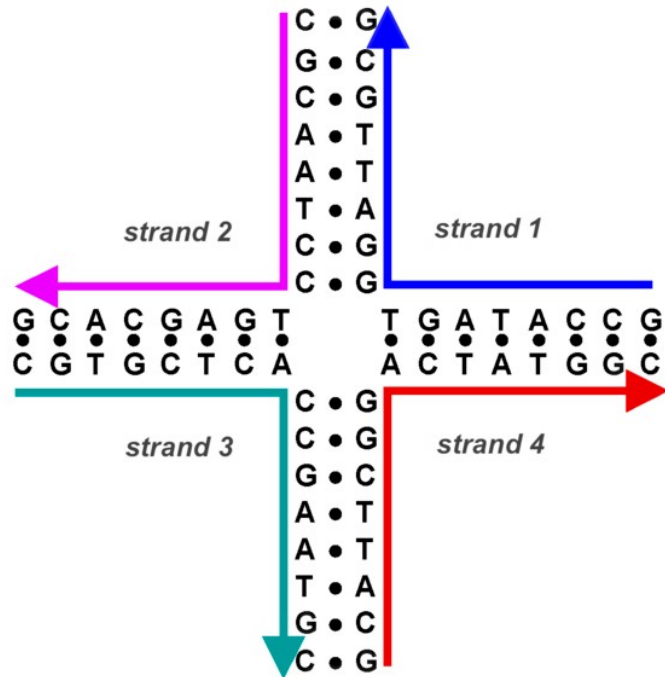
Venkatraman
Ramakrishnan



The [Nobel Prize in Chemistry](#).
2009

šaltiniai: Vikipedija, Baltymų duomenų bankas (PDB)

RNR antrinių struktūrų spėjimas



http://en.wikipedia.org/wiki/RNA_structure

http://en.wikipedia.org/wiki/List_of_RNA_structure_prediction_software