The structure of RNA is as varied as its functions. The single-stranded RNA molecule often folds back on itself to form double-helical stem capped by a loop of non-Watson-Crick paired or unpaired nucleotides of various sizes, which are thought to provide tertiary recognition sites for both proteins and nucleic acids.

The four-base loops cap many double-helical structures in rRNA. Although 256 different tetraloop sequences are possible, nearly 70% of all the four-base loops in rRNAs are either UNCG or GNRA (where N is any nucleotide and R is a purine), with extraordinary high melting temperatures in comparison with similar RNA sequences (Woese et al. 1990).

The goal of our MDS was to make clear remaining questionable structural features of the UACG tetraloop in the very short hairpin (Abdekalifi et al. 1997), for which an
experimental research produces either inconsistent results (the rA residue conformation),
or determination of which is beyond capabilities of contemporary experimental appar­
tuses (the mode of the hydrogen bond connection in the atypical terminal iU-rG pair of
residues in the tetraloop) Except it, we were interested in the influence of 2′hydroxyls
groups on the stabilization of the hairpin structure due to the creation of hydrogen bonds,
either in the mentioned iU-rG terminal pair of residues or elsewhere, because it seems to
be the reason of the substantially higher thermodynamic stability of UNCG tetraloops in
comparison with then deoxyoligonucleotide analogues

In our MDS the hairpin structure seemed to be stable in the temperature range
up to 285 K with the rA residue in the C3endo/anti conformation. In the case of higher
temperatures the C3endo/anti conformation of the rA residue changed to the C2endo/syn
conformation

One hydrogen bond between RU and rG bases and the other between the RU 2′hy­
droxyl group and the rG base stable in both C3endo/anti and C2endo/syn conformations
(proposed on the base of NMR results (Allam and Varam 1995) established in the course of
our fully solvated MDS. This kind of the hydrogen bond connection gives the explanation
of higher stability of RNA loops in comparison with the same deoxy-sequences

We found also three other supplementary hydrogen bonds, which formed between
2′hydroxyl and site phosphate groups (in the stem in two cases and once in the loop
sequence of the hairpin)

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X-Ray Crystal Structure of GpC phosphonate Analogue:
A Promising Unit for the SNAIGE Strategy

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Key words: SNAIGE concept, crystal structure, GpC phosphonate analogue

Several new concepts called, as a whole, the SNAIGE concept (Synthetic Nucleic
Acids Interfering with Gene Expression), have been introduced into chemotherapy in
recent period of time, such as the idea of “antisense” oligonucleotides

The first X-ray crystal structure of novel-type diribonucleoside monophosphate ana­
logues, the crystal structure of (guanosine-2′-O-phosphonomethyl)-5′-O-cytidine (G-p>C
2′) was determined. Structural unit involves two asymmetric molecules of G-p>C, Mg2+
and 13 H2O, differing in conformation of phosphonate analog of phosphodiester linkage