

## Poster Presentation

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### *Crystal structure of unusual RNA duplex containing strontium ion binding motif*

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Crystal structures of several functional non-coding RNAs, such as ribozymes, aptamers, ribosomes and tRNAs, have been reported so far. Unusual structural motifs and non-complementary base pairs are important for their functions. In the present study, we have determined a crystal structure of an unusual RNA duplex containing a strontium ion binding motif. A 19 mer RNA (5'-UUGUCGCUU[Br]CGAAAAAGUC-3') was chemical synthesized and purified by denaturing PAGE. Crystallizations were performed by the sitting-drop vapor diffusion method. The initial phase was solved by the SAD method. Atomic parameters were refined at a resolution of 3.0 Å. The 19 mer RNA forms an unusual antiparallel duplex. At both ends of the duplex, the Watson-Crick G=C and A-U and the Wobble GoU and AoC base pairs are formed. The Wobble C10oA14\* pair is available only in acidic condition by protonation of N1 of A14\* (\* indicates residues of the opposite strand). Two hydrogen bonds, N1-H(A14\*)...O2(C10) and N6-H(A14\*)...N3(C10), are observed in the base pair. In the center of the duplex, two sheared G11oA13\* and G11\*oA13 base pairs are formed. The distance between two RNA chains becomes shorter by the GoA base pair and hydrogen bonds between the Watson-Crick edge of G11 and the phosphate group of A12\*. Therefore, the central A12 residue cannot make a base pair, but it makes a stacking interaction with A12\*. The A12 residue stacks also with A13 of the sheared GoA base pair. As a result, an A13-A12-A12\*-A13\* stacked column is formed at the minor groove of the duplex, and the G11 base of the sheared GoA base pair is inclined toward the minor groove. By taking such a unique structure, the RNA duplex has a Sr<sup>2+</sup> ion binding pocket in the center. A hydrated Sr<sup>2+</sup> ion binds to O6 and N7 of G11 and G11\*. The Sr<sup>2+</sup> ion is surrounded by four phosphate groups of two RNA chains. The Sr<sup>2+</sup> ion is tightly captured by eight hydrogen bonds in total.

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