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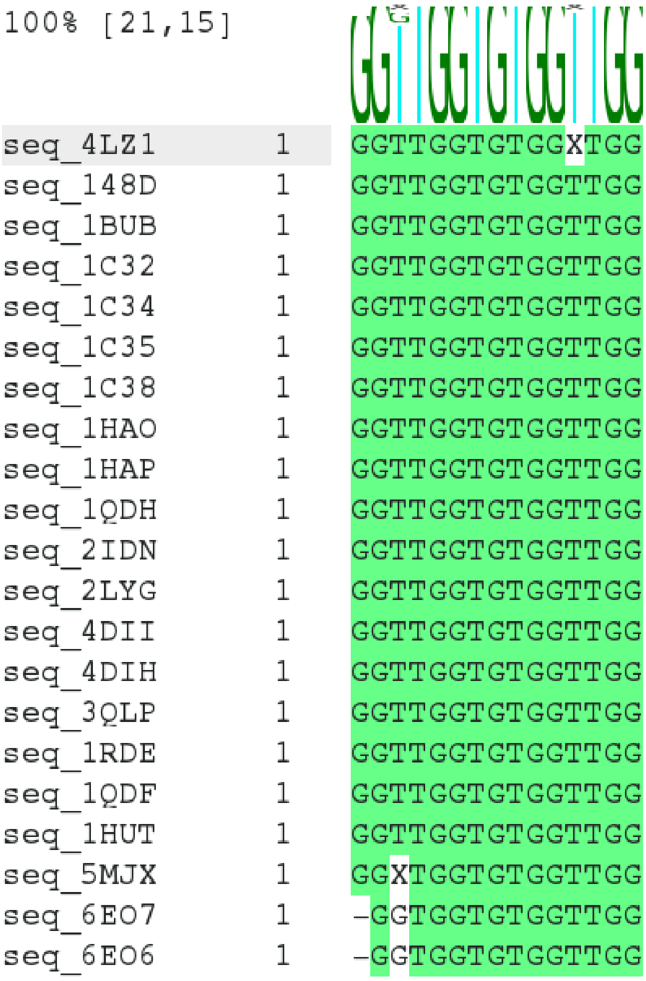
Supplementary Materials

Analysis of sequence motives in G-quadruplex folding groups

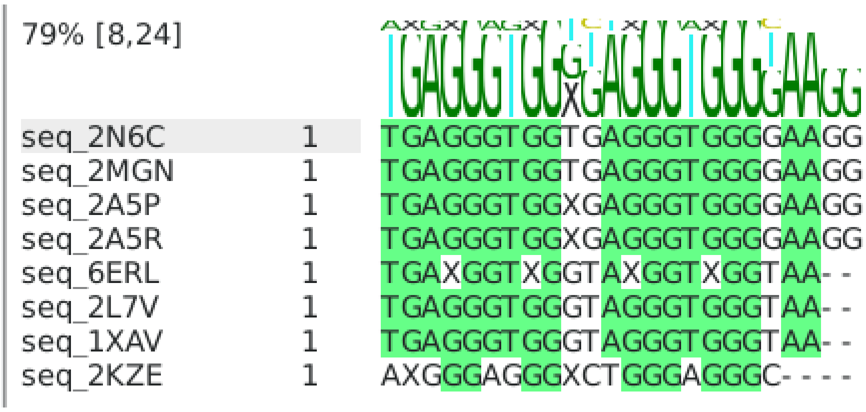
We performed the multiple alignment analysis of the aptamer sequences, for the most populated folding type (Supplementary Figs. S1-S3). The analysis was performed using Align tool in ICM-pro software package (http://www.molsoft.com/icm_pro.html) and was applied for single-stranded aptamers from folding groups 2,3,6 and 9 (Fig. 4), as the most populated folding types, observed in available crystal structures. To improve the quality of multiple sequence analysis we excluded sequences, forming gaps. Resulted alignment for folding type 6 (“unimolecular chair”) was formed by 21 sequences and sequence similarity score of 100% (Supplementary Fig. S1); alignment of sequences from folding type 3 consist of 8 sequences, sequence similarity score 79% (Supplementary Fig. S2); we combined alignment for groups 2 and 9, since they consist of aptamers with very close sequences, the resulted alignment consists of 35 sequences with score of 78% (Supplementary Fig. S3).



```
100% [21,15]

seq_4LZ1    1   GGTTGGTGTGGXTGG
seq_148D    1   GGTTGGTGTGGTTGG
seq_1BUB    1   GGTTGGTGTGGTTGG
seq_1C32    1   GGTTGGTGTGGTTGG
seq_1C34    1   GGTTGGTGTGGTTGG
seq_1C35    1   GGTTGGTGTGGTTGG
seq_1C38    1   GGTTGGTGTGGTTGG
seq_1HAO    1   GGTTGGTGTGGTTGG
seq_1HAP    1   GGTTGGTGTGGTTGG
seq_1QDH    1   GGTTGGTGTGGTTGG
seq_2IDN    1   GGTTGGTGTGGTTGG
seq_2LYG    1   GGTTGGTGTGGTTGG
seq_4DII    1   GGTTGGTGTGGTTGG
seq_4DIH    1   GGTTGGTGTGGTTGG
seq_3QLP    1   GGTTGGTGTGGTTGG
seq_1RDE    1   GGTTGGTGTGGTTGG
seq_1QDF    1   GGTTGGTGTGGTTGG
seq_1HUT    1   GGTTGGTGTGGTTGG
seq_5MJX    1   GGXTGGTGTGGTTGG
seq_6EO7    1   -GGTGGTGTGGTTGG
seq_6EO6    1   -GGTGGTGTGGTTGG
```

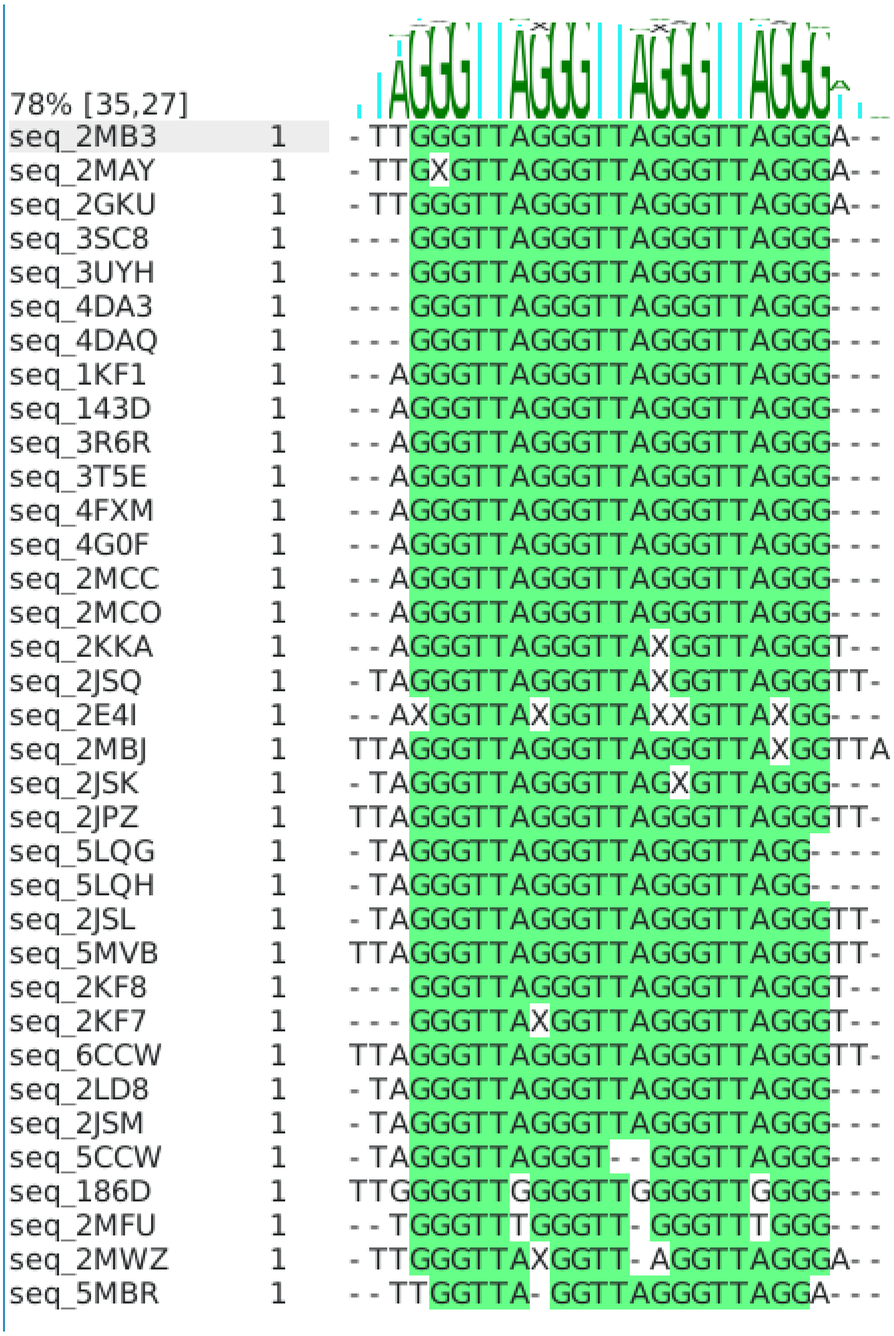
Supplementary Figure S1 Multiple alignment analysis of aptamer sequences having folding type 6 (“unimolecular chair”).



```
79% [8,24]

seq_2N6C    1   TGAGGGTGGTGAGGGTGGGGAAGG
seq_2MGN    1   TGAGGGTGGTGAGGGTGGGGAAGG
seq_2A5P    1   TGAGGGTGGXGAGGGTGGGGAAGG
seq_2A5R    1   TGAGGGTGGXGAGGGTGGGGAAGG
seq_6ERL    1   TGAXGGTXGGTAXGGTXGGTAA--
seq_2L7V    1   TGAGGGTGGGTAGGGTGGGTAA--
seq_1XAV    1   TGAGGGTGGGTAGGGTGGGTAA--
seq_2KZE    1   AXGGGAGGGXCTGGGAGGGC----
```

Supplementary Figure S2 Multiple alignment analysis of aptamer sequences having folding type 3.



```
78% [35,27]
seq_2MB3   1   -TTGGGTTAGGGTTAGGGTTAGGGA--
seq_2MAY   1   -TTGXGTTAGGGTTAGGGTTAGGGA--
seq_2GKU   1   -TTGGGTTAGGGTTAGGGTTAGGGA--
seq_3SC8   1   ---GGGTTAGGGTTAGGGTTAGGG---
seq_3UYH   1   ---GGGTTAGGGTTAGGGTTAGGG---
seq_4DA3   1   ---GGGTTAGGGTTAGGGTTAGGG---
seq_4DAQ   1   ---GGGTTAGGGTTAGGGTTAGGG---
seq_1KF1   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_143D   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_3R6R   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_3T5E   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_4FXM   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_4G0F   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_2MCC   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_2MCO   1   --AGGGTTAGGGTTAGGGTTAGGG---
seq_2KKA   1   --AGGGTTAGGGTTAXGGTTAGGGT--
seq_2JSQ   1   -TAGGGTTAGGGTTAXGGTTAGGGTT-
seq_2E4I   1   --AXGGTTAXGGTTAXXGTTAXGG---
seq_2MBJ   1   TTAGGGTTAGGGTTAGGGTTAXGGTTA
seq_2JSK   1   -TAGGGTTAGGGTTAGXGTTAGGG---
seq_2JPZ   1   TTAGGGTTAGGGTTAGGGTTAGGGTT-
seq_5LQG   1   -TAGGGTTAGGGTTAGGGTTAGG----
seq_5LQH   1   -TAGGGTTAGGGTTAGGGTTAGG----
seq_2JSL   1   -TAGGGTTAGGGTTAGGGTTAGGGTT-
seq_5MVB   1   TTAGGGTTAGGGTTAGGGTTAGGGTT-
seq_2KF8   1   ---GGGTTAGGGTTAGGGTTAGGGT--
seq_2KF7   1   ---GGGTTAXGGTTAGGGTTAGGGT--
seq_6CCW   1   TTAGGGTTAGGGTTAGGGTTAGGGTT-
seq_2LD8   1   -TAGGGTTAGGGTTAGGGTTAGGG---
seq_2JSM   1   -TAGGGTTAGGGTTAGGGTTAGGG---
seq_5CCW   1   -TAGGGTTAGGGT--GGGTTAGGG---
seq_186D   1   TTGGGGTTGGGGTTGGGGTTGGGG---
seq_2MFU   1   --TGGGTTTGGGTT-GGGTTTGGG---
seq_2MWZ   1   -TTGGGTTAXGGTT-AGGTTAGGGA--
seq_5MBR   1   --TTGGTTA-GGTTAGGGTTAGGA---
```

Supplementary Figure S3 Joined multiple alignments of aptamer sequences having folding types 2 and 9.