Aptamers
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SUPPLEMENTARY DATA

MINIREVIEW

Conformational flexibility and structural dynamics of aptamers

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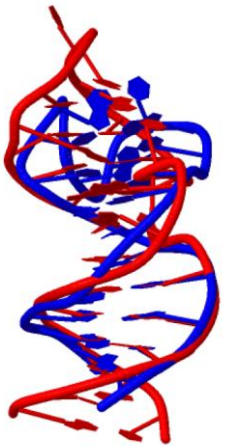
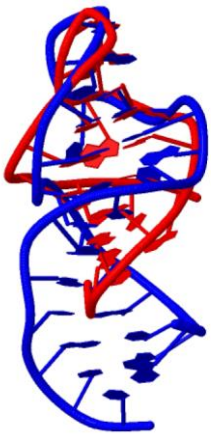
Supplementary Table 1. Structural alignment of selected examples of aptamers of different sequences that bind to the same target ligand. According to Zhang and co-workers (Gong et al, 2019), 'alignment' was carried out based on the distance between nucleotide pairs in the two sequences, while 'superposition' was the overlay of two structures via rotation and translation operations to maximize the template modeling score. ":" represents residue pairs of distance smaller than 5.0 Å, and "." represents other aligned residues.

Aptamer sequence alignment (5' → 3')	**Superimposed structures**
Arginine-binding aptamers (originally selected by Harada and Frankel, 1995)	

1OLD d(GATCGAAACGTAGCGCCTTCGATC) (Lin and Patel, 1996)
 	
2ARG d(TGACCAGGGCAAACGGTAGGTGAGTGGTCA) (Lin et al, 1998)
 	
`--gatcgaa-acgtagcg----ccttcgatc--`
`  ::::::: :: :  .:    :::::::::`
`tgaccagggcaa-a--cggtaggtgagtggtca`
RMSD = 2.63 Å
	
	(Superposition between structures 2 and 9 from 1OLD and 2ARG, respectively) Blue: 1OLD; Red: 2ARG

Tobramycin-binding aptamers (originally selected by Wang and Rando, 1995)	

1TOB r(GGCACGAGGUUUAGCUACACUCGUGCC)
(Jiang et al, 1997)
 	
2TOB r(GGGACUUGGUUUAGGUAAUGAGUCCC)
(nucleotides in red are not included in the resolved DNA structures) (Jiang and Patel, 1998)
`ggcac--gagguuuagcuacacucgugcc-----`
`       ::::::::::::`
`-----acuugguuuagguaa---------ugagu`
 	
RMSD = 1.40 Å
	
	(Superposition between structures 2 and 4 from 1TOB and 2TOB, respectively) Blue: 1TOB; Red: 2TOB

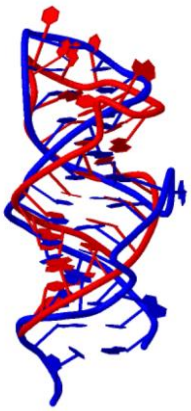
HIV-1 Rev peptide (selection originally described by Giver et al, 1993)

1ULL r(GGCUGGACUCGUACUUCGGUACUGGAGAAACAGCC) (Ye et al, 1996)

484D r(GGUGUCUUGGAGUGCUGAUCGGACACC)
(Ye et al, 1999)

```
ggcuggacuc-g-uacuucgguacuggagaaacagcc
     :::::: : :::::::::::: :: : :::
----ggugucuuggagugcugaucg-ga-c-acc---
```

RMSD=2.42 Å



(Superposition between structures 2 and 17 from 1ULL and 484D, respectively) Blue: 1ULL; Red: 484D

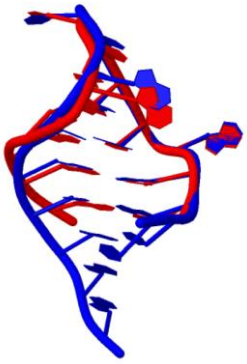
Aptamer against bacteriophage MS2 coat protein

5MSF r(CCGGAGGAUCACCACGGG) (Rowsell et al, 1998)
6MSF r(CCACAGUCACUGGG) (Convery et al, 1998)
7MSF r(UCGCCAACAGGCGG) (Rowsell et al, 1998)

5MSF and 6MSF

```
ccggaggaucaccacggg
  ::::::::::::::
--ccacagucacuggg--
```

RMSD = 1.72 Å

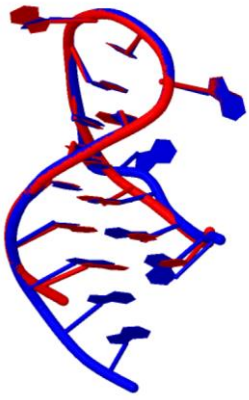


Superposition between 5MSF (blue) and 6MSF (red)

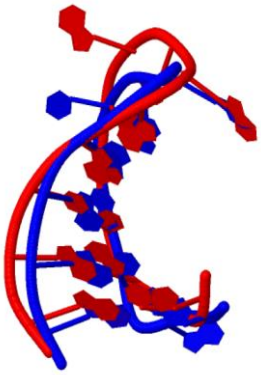
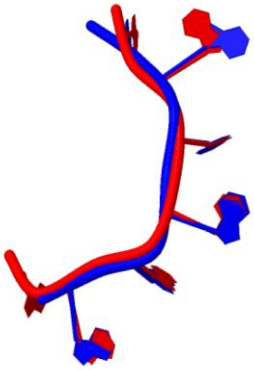
5MSF and 7MSF

```
ccggaggaucaccacggg
 ::: ::::::::::::
-ucg-ccaacaggcgg--
```

RMSD = 0.72 Å



Blue: 5MSF; Red: 7MSF

6MSF and 7MSF ccacagu-cacuggg :: :::: ::::::: uc-gccaacaggcgg RMSD = 1.27 Å	 Blue: 6MSF; Red: 7MSF
Hfq from *Bacillus subtilis*	
3HSB r(AGAGAGA) (Someya et al, 2012) 3AHU r(AGAGAG) (Someya et al, 2012) agagag- :::::: Agagaga RMSD = 0.39 Å	 Superposition between 3HSB (red) and 3AHU (blue)

[a]RMSD calculated using RNA-align (https://zhanggroup.org/RNA-align/) (Gong et al, 2019). In the cases of structures determined by NMR as ensembles, alignment and superposition were performed for the structures closest to the average as determined by the WHAT IF server (https://swift.cmbi.umcn.nl/servers/html/index.html) developed by Gert Vriend at the Centre for Molecular and Biomolecular Informatics of Radboud University, Netherland.