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Supplementary data

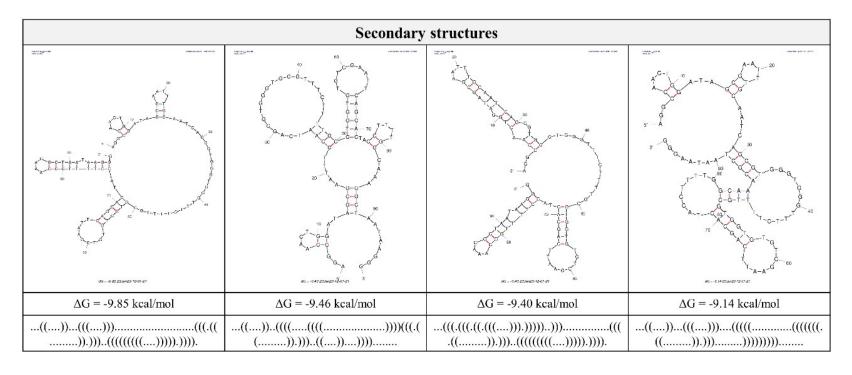


Figure S1. Possible secondary structures of Apt5 predicted by mFold software.

Secondary/ tertiary structure	1	2	3	4	5	6	7	8	9	10
A										
В										
C										
D										

Figure S2. Predictions of the three-dimensional structures of all Apt5 secondary structures as well as their docking with the target molecule, SEA. The tertiary structures of the aptamer were predicted by the 3dRNA webserver and docking by the HDOCK webserver.

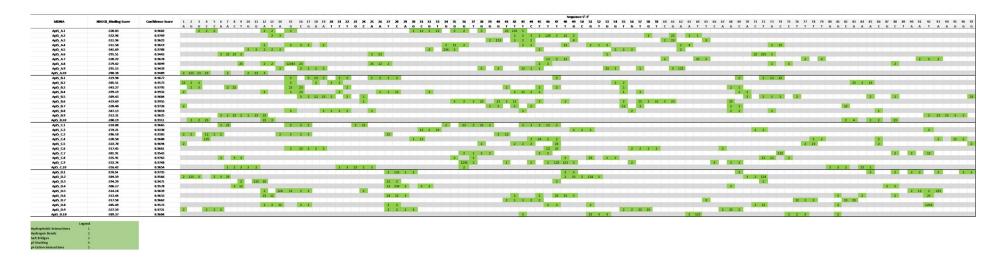


Figure S3. Analysis of all predictions of the original Apt5 showing the interaction residuals (in green) as well as the type of physicochemical interaction with SEA according to the PLIP web tool.

LNA 1	LNA 2	LNA 3	LNA 4	LNA 5	LNA 6	LNA 7	LNA 8	LNA 9	LNA 10	LNA 11	
			The state of the s								
LNA 12	LNA 13	LNA 14	LNA 15	LNA 16	LNA 17	LNA 18	LNA 19	LNA 20	LNA 21		

Figure S4. Predictions of the three-dimensional structures of LNA versions as well as their docking with the target molecule, SEA. The tertiary structures correspond to the most likely structure of the original Apt5 modified with LNA using BIOVIA software and docking by HDOCK webserver.

Aptemer variation	Nudeotides with LNA modifications	3dRNA/QRNAS	HDOCK		1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 93											92 93 94 95 96 97			
		RMSD (Å)	Binding Score	Confidence S	core AGGCCAACTGGATAGC	GAATTT	GCAATCA	G C G T G G G T G	GGTTT	CTTT	TGCG	T G G T G T G	TCGAA	TCAGC	ACTACO	TTTTG	GCAAAC	GCTAA	TAAGGG
Apt5_DNA_8.6 (original)	Original		-419.69	0.9955			2	3 2 2 23	23 2 1	2	1	2 23 2	12 3 23	23					
Apt5_LNA1	1	0,157	-409.50	0.9945			2	3 2 2 23	23 2 12	2	1	2 2 2	12 3 23	23					
Apt5 LNA2	1,2	0,129	-370.25	0.9879	2 2 2	2 2 23	2 2 25			2 2		1		2	3				
Apt5_LNA3	1,2,3	0,260	-415.44	0.9951			2	3 2 12 23	23 2 12	2	1	2 2 2	12 23 23	23					
Apt5_LNA4	95, 96, 97	0,104	-385.00	0.9910			2	3 2 12 23	23 12			12 2 2	12 23	23					
Apt5 LNAS	96, 97	0,103	-355.84	0.9840			2	3 2 12 123	23 2 12			12	12 23	2					
AptS_LNA6	97	0,109	-410.49	0.9946			2	3 2 12 23	23 2 12	2	1	2 2 2	12 3 23	23					
Apt5_UNA7	87	0,106	-403.07	0.9937			2	3 2 12 23	23 2 12	2		2 2 2	12 23	123					
Apt5_LNA8	88	0,107	-375.97	0.9892			2	3 2 12 23	23 2 1			12 2 2	12 23	23					
Apt5 LNA9	16	0,125	-411.06	0.9946			2	3 2 12 23	23 2 1	2	1	2 2 2 2	12 23 23	23					
Apt5_LNA10	15	0,182	-390.70	0.9919			2	23 2 12 23	2 2 12	2		2	12 3 23	23					
Apt5_LNA11	15, 87	0,114	-385.32	0.9910			2	3 2 2 23	23 2 12			12 2 2	12 3 23	23					
Apt5_UNA12	16, 88	0,126	-397.27	0.9929			2	2 2 2 23	23 2 2 2	2	1	2 2 2	12 23	23					
Apt5_LNA13	1, 2, 3, 95, 96, 97	0,172	-388.96	0.9917			2	23 2 12 23	2 2 12			2 2 2	12 23 23 1	23					
Apt5_UNA14	1, 2, 3, 15, 87, 95, 96, 97	0,174	-401.24	0.9935			2	3 2 12 23	23 2 12	2		12 2 2	12 3 23	123					
Apt5_LNA15	1, 2, 3, 16, 88, 95, 96, 97	0,266	-388.82	0.9916			2	2 2 2 23	23 2 2	12	12	2 2 2	12 3 23	123					
Apt5_LNA16	23	0,236	-415.40	0.9951			2	3 2 12 23	23 2 12	12	12	2 2 2	12 3 23	23					
Apt5_UNA17	50	0,314	-402.04	0.9936			2	3 2 12 23	23 2 12	2 2		2 2 2	12 23	123					
Apt5_LNA18	23, 50	0,179	-376.49	0.9893			2	3 2 12 123	2 2 12	2	2	12 12	12 3 23	23					
Apt5_LNA19	54	0,128	-379.19	0.9899			2	2 2 2 23	23 2 2	12	1	2 2 2 2	12 3 23	123					
AptS_LNA20	67	0,285	-391.70	0.9921			2	23 2 2 23	23 2 2 2	2 2	12	2 2 2 2	12 23	23					
Apt5_LNA21	54, 67	0,272	-374.48	0.9889			2	3 2 12 123	2 12 2	2		12 2 2 2	12 23	123					

Figure S5. Analysis of all predictions of the original Apt5 showing the interaction residuals (in green) as well as the type of physicochemical interaction with SEA according to the PLIP web tool.