Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.
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Supplementary data

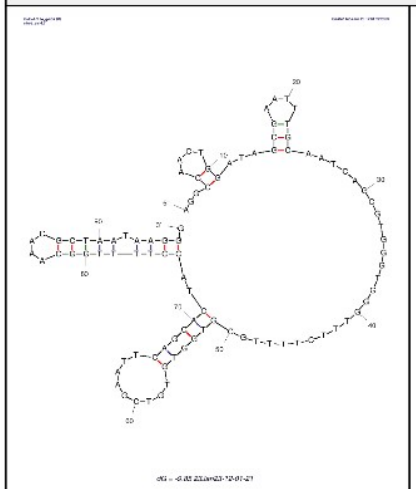
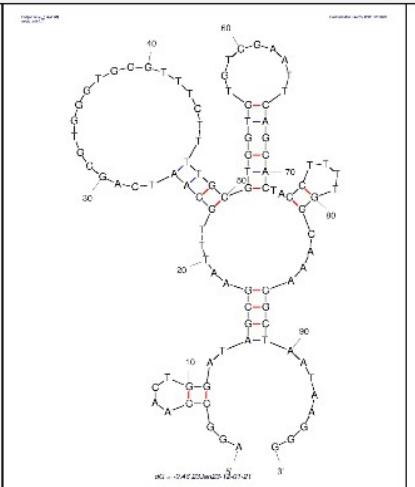
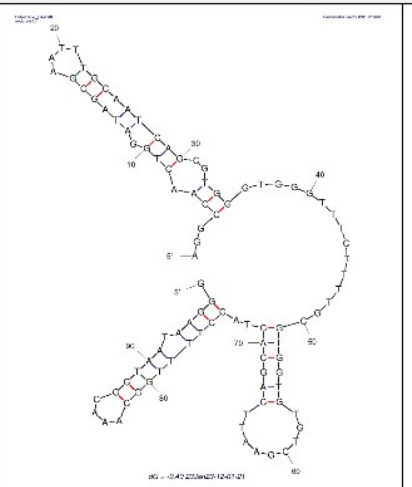
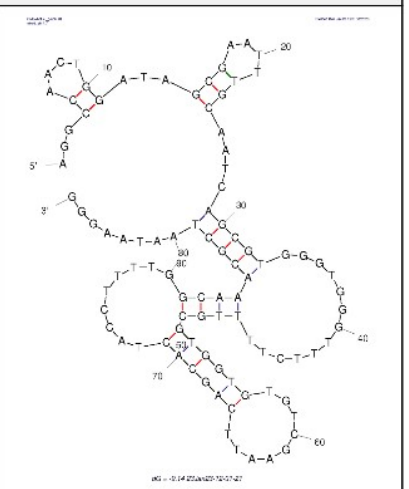
Secondary structures			
			
ΔG = -9.85 kcal/mol	ΔG = -9.46 kcal/mol	ΔG = -9.40 kcal/mol	ΔG = -9.14 kcal/mol
...((....))...(((....)))..... (((.((.....)).)))..((((((((....)))))).)))).	...((....))..((((.....((((.....))))(((.((.....)).)))..((....))....))).....	...(((.(((.((.(((....))).)))))..))).....(((.((.....)).)))..((((((((....)))))).)))).	...((....))...(((....)))....((((.....((((((. ((.....)).))).....))))))).....

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

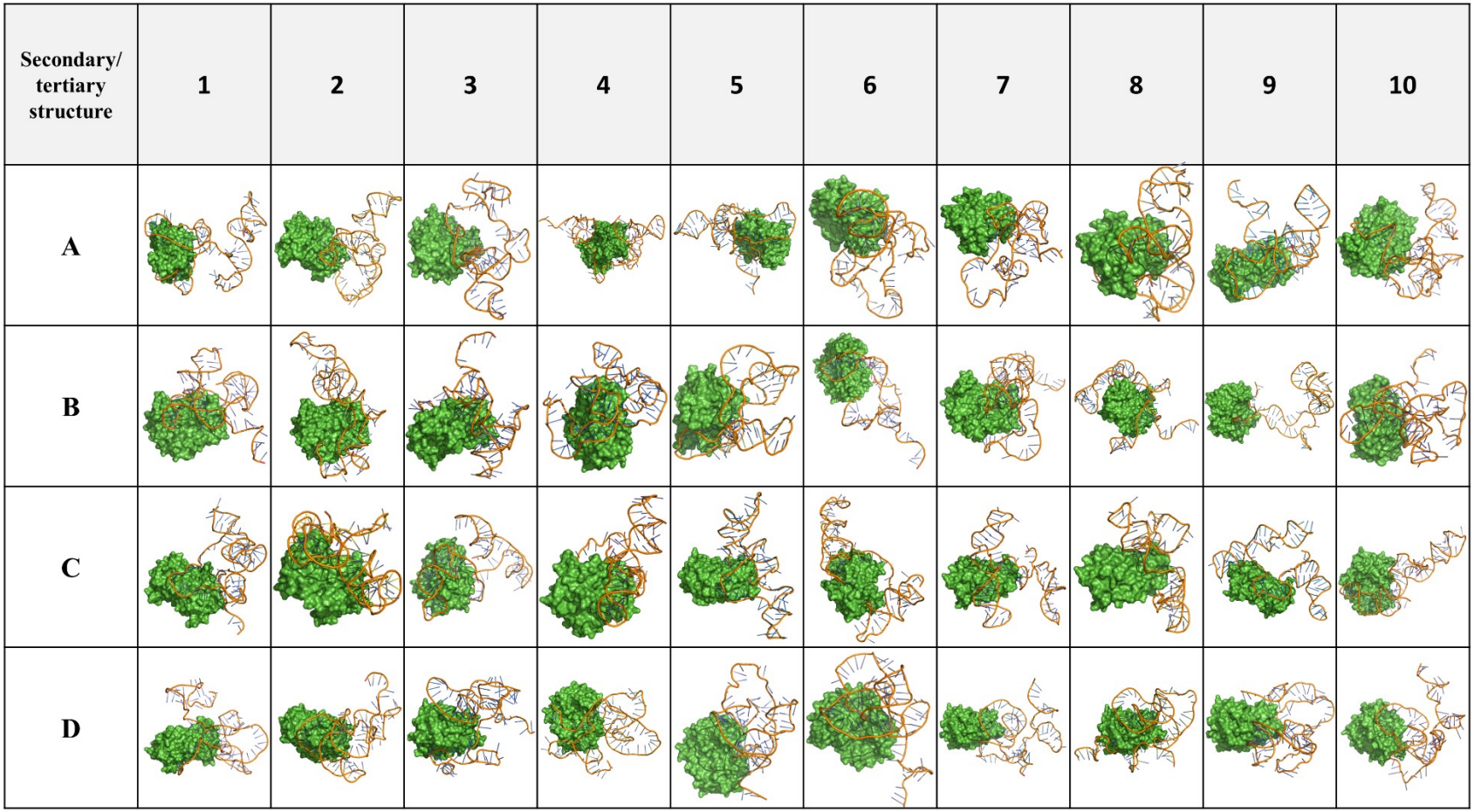


Figure S2. Predictions of the three-dimensional structures of all Apt5 secondary structures as well as their docking with the target molecule, SEA. The tertiary structures of the aptamer were predicted by the 3dRNA webserver and docking by the HDOCK webserver.

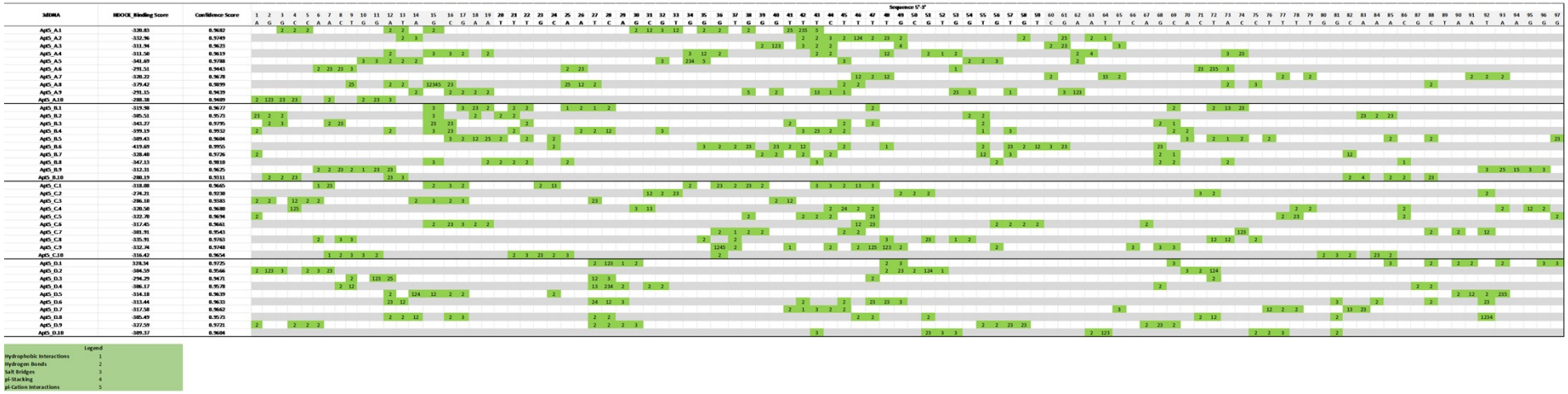


Figure S3. Analysis of all predictions of the original Apt5 showing the interaction residuals (in green) as well as the type of physicochemical interaction with SEA according to the PLIP web tool.

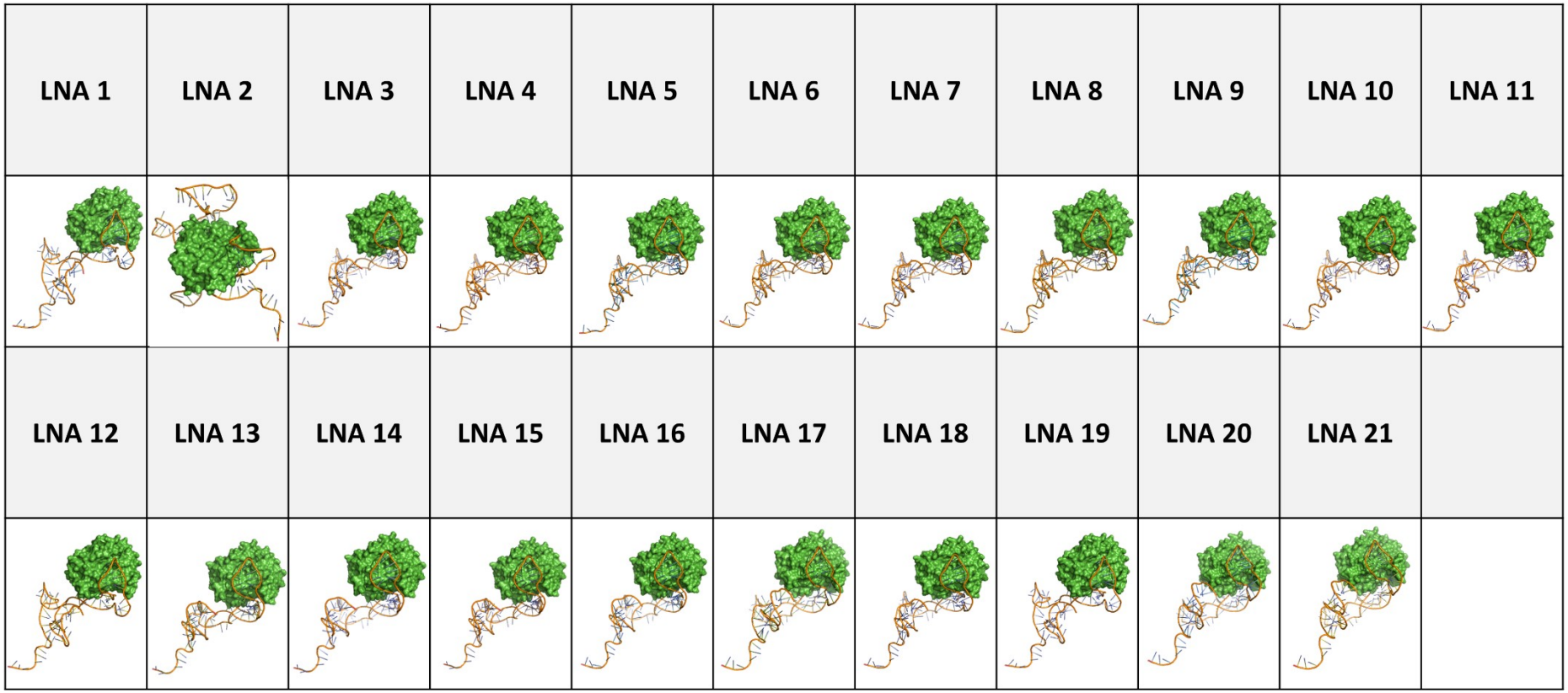


Figure S4. Predictions of the three-dimensional structures of LNA versions as well as their docking with the target molecule, SEA. The tertiary structures correspond to the most likely structure of the original Apt5 modified with LNA using BIOVIA software and docking by HDOCK webserver.

Aptamer variation	Nucleotides with LNA modifications	3dRNA/QRNAS RMSD (Å)	HDOCK Binding Score	HDOCK Confidence Score
Apt5_DNA_B.6 (original)	Original	-	-419.69	0.9955
Apt5_LNA1	1	0,157	-409.50	0.9945
Apt5_LNA2	1, 2	0,129	-370.25	0.9879
Apt5_LNA3	1, 2, 3	0,260	-415.44	0.9951
Apt5_LNA4	95, 96, 97	0,104	-385.00	0.9910
Apt5_LNA5	96, 97	0,103	-355.84	0.9840
Apt5_LNA6	97	0,109	-410.49	0.9946
Apt5_LNA7	87	0,106	-403.07	0.9937
Apt5_LNA8	88	0,107	-375.97	0.9892
Apt5_LNA9	16	0,125	-411.06	0.9946
Apt5_LNA10	15	0,182	-390.70	0.9919
Apt5_LNA11	15, 87	0,114	-385.32	0.9910
Apt5_LNA12	16, 88	0,126	-397.27	0.9929
Apt5_LNA13	1, 2, 3, 95, 96, 97	0,172	-388.96	0.9917
Apt5_LNA14	1, 2, 3, 15, 87, 95, 96, 97	0,174	-401.24	0.9935
Apt5_LNA15	1, 2, 3, 16, 88, 95, 96, 97	0,266	-388.82	0.9916
Apt5_LNA16	23	0,236	-415.40	0.9951
Apt5_LNA17	50	0,314	-402.04	0.9936
Apt5_LNA18	23, 50	0,179	-376.49	0.9893
Apt5_LNA19	54	0,128	-379.19	0.9899
Apt5_LNA20	67	0,285	-391.70	0.9921
Apt5_LNA21	54, 67	0,272	-374.48	0.9889

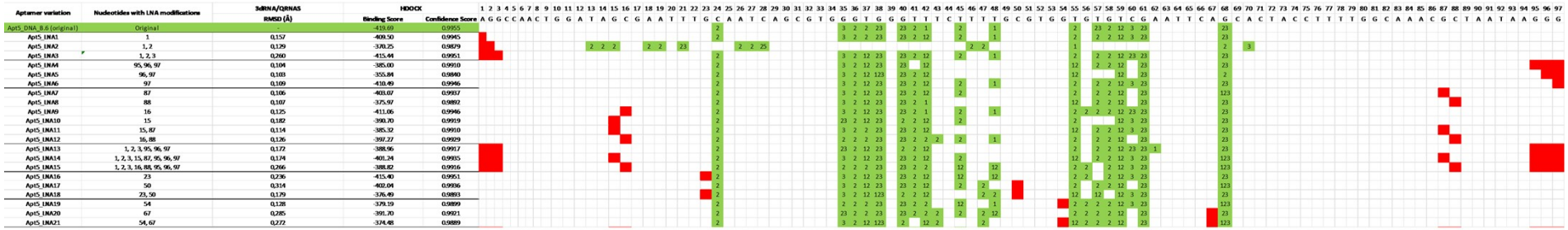


Figure S5. Analysis of all predictions of the original Apt5 showing the interaction residuals (in green) as well as the type of physicochemical interaction with SEA according to the PLIP web tool.