SUPPLEMENTARY MATERAL

Analysis of the αCP1-KH3-poly(C)RNA model

Following are tables describing the oligonucleotide stereochemistry and hydrogen bonding interactions that occur during the molecular dynamics simulation of the αCP1-KH3/8-nt poly(C)-RNA model as described in the manuscript.

Sterochemistry of modelled RNA

The backbone dihedral angles of the poly(C)-RNA in the αCP1-KH3-RNA model were calculated at every picosecond timestep in the 1 ns molecular dynamics simulation. The mean and std deviation (second and third value in each cell) of these angles are listed and allow the degree of movement over the simulation as well as any departure from the original model (first value - in bold) to be noted. The six dihedral angles which describe the oligonucleotide backbone are defined (as per standard nomenclature) by the following atoms:

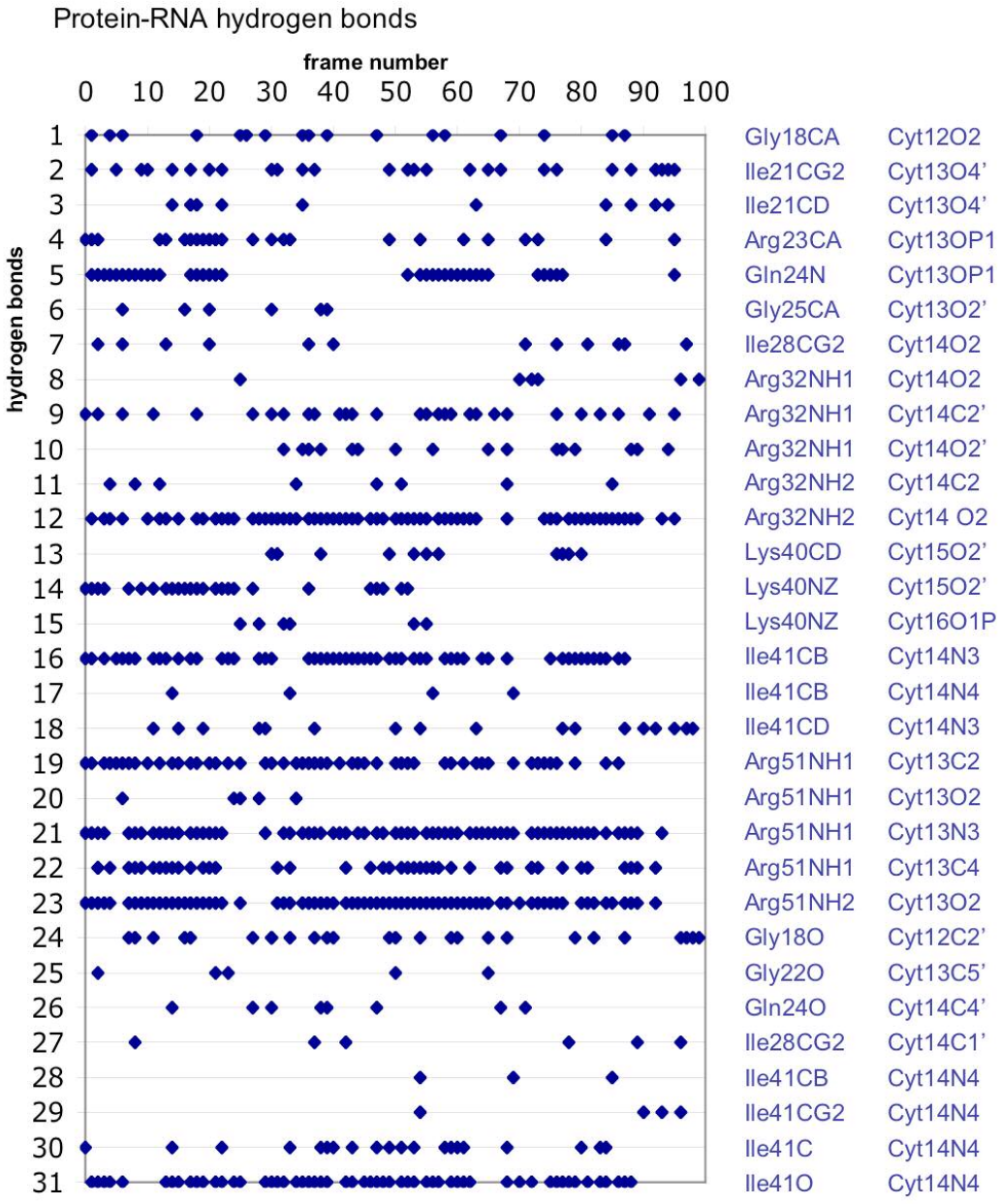
alpha:	-O3'	P	O5'	C5'
beta:	P	O5'	C5'	C4'
gamma:	O5'	C5'	C4'	C3'
delta:	C5'	C4'	C3'	O3'
epsilon:	C4'	C3'	O3'	+P
zeta:	C3'	O3'	+P	+O5'

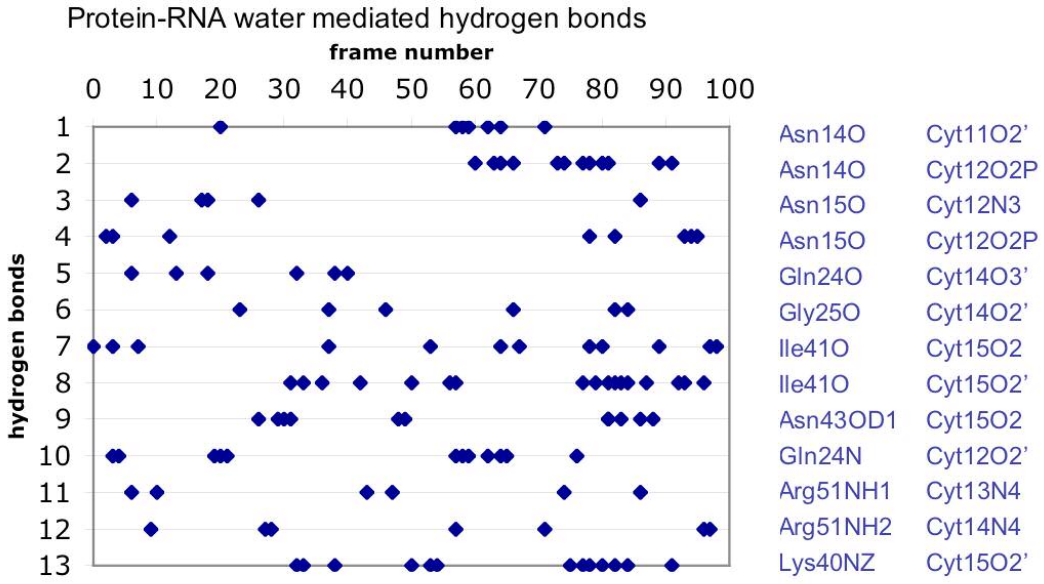
Base*	alpha	beta	gamma	delta	epsilon	zeta
9	N/A	**173.7**	**43.0**	**85.8**	**66.6**	**-57.2**
		23.8	60.10	75.8	-65.4	94.7
		149.5	13.02	6.4	142.0	94.7
10	**-127.5**	**170.7**	**93.0**	**105.5**	**-127.8**	**-60.9**
	-31.5	100.9	51.5	141.7	-112.6	-77.4
	61.0	99.3	19.0	7.9	16.7	17.3
11	**124.9**	**137.9**	**42.8**	**118.6**	**-76.2**	**165.4**
	109.2	92.7	57.2	139.5	-116.9	-110.5
	30.8	130.8	14.9	7.4	31.3	15.0
12	**-102.4**	**160.9**	**40.11**	**92.9**	**79.4**	**98.8**
	-72.9	130.0	38.1	74.9	39.7	8.8
	18.7	34.8	15.1	5.9	8.7	169.2
13	**111.3**	**-110.8**	**133.3**	**112.7**	**-112.4**	**132.7**
	-62.2	146.2	30.2	146.5	-103.0	123.2
	27.0	51.4	25.0	6.6	18.4	19.3
14	**-76.9**	**143.5**	**37.7**	**78.5**	**-135.7**	**-60.0**
	-105.0	145.1	53.8	78.1	105.9	25.5
	22.2	27.6	11.0	5.7	127.0	16.3
15	**-63.8**	**179.5**	**48.7**	**82.1**	**-132.9**	**-63.9**
	-131.5	74.3	64.0	79.7	-86.1	-33.2
	14.1	155.6	9.6	5.2	102.6	31.0
16	**-65.2**	**172.5**	**51.0**	N/A	N/A	N/A
	-82.6	99.5	59.8			
	29.7	133.2	10.7			

* the numbering system is based on the oligonucleotide numbering within the Nova2-KH3-RNA structure (accession code: 1EC6) with bases **12-15** corresponding to the binding tetrad.

Hydrogen bonding

The lifetime of potentially important hydrogen bond interactions occurring between the protein and oligonucleotide assessed by determining their existence at each picosecond of the 1 ns molecular dynamics simulation (shown as a dot at each timepoint). Their presence was defined by the hydrogen bond acceptor and donor occurring within 3.8 Å of one another and within an X-H-X angle of 30^{o} degrees where X = the heavy atom. Water mediated hydrogen bonds occurring between the protein and oligonucleotide were defined as simultaneous hydrogen bonds occurring between the protein and the oligonucleotide to the same water oxygen.





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