Supplemental Data

Selection of 2'-Deoxy-2'-Fluoroarabino Nucleic Acid (FANA) Aptamers that Bind HIV-1 Integrase with Picomolar Affinity

By

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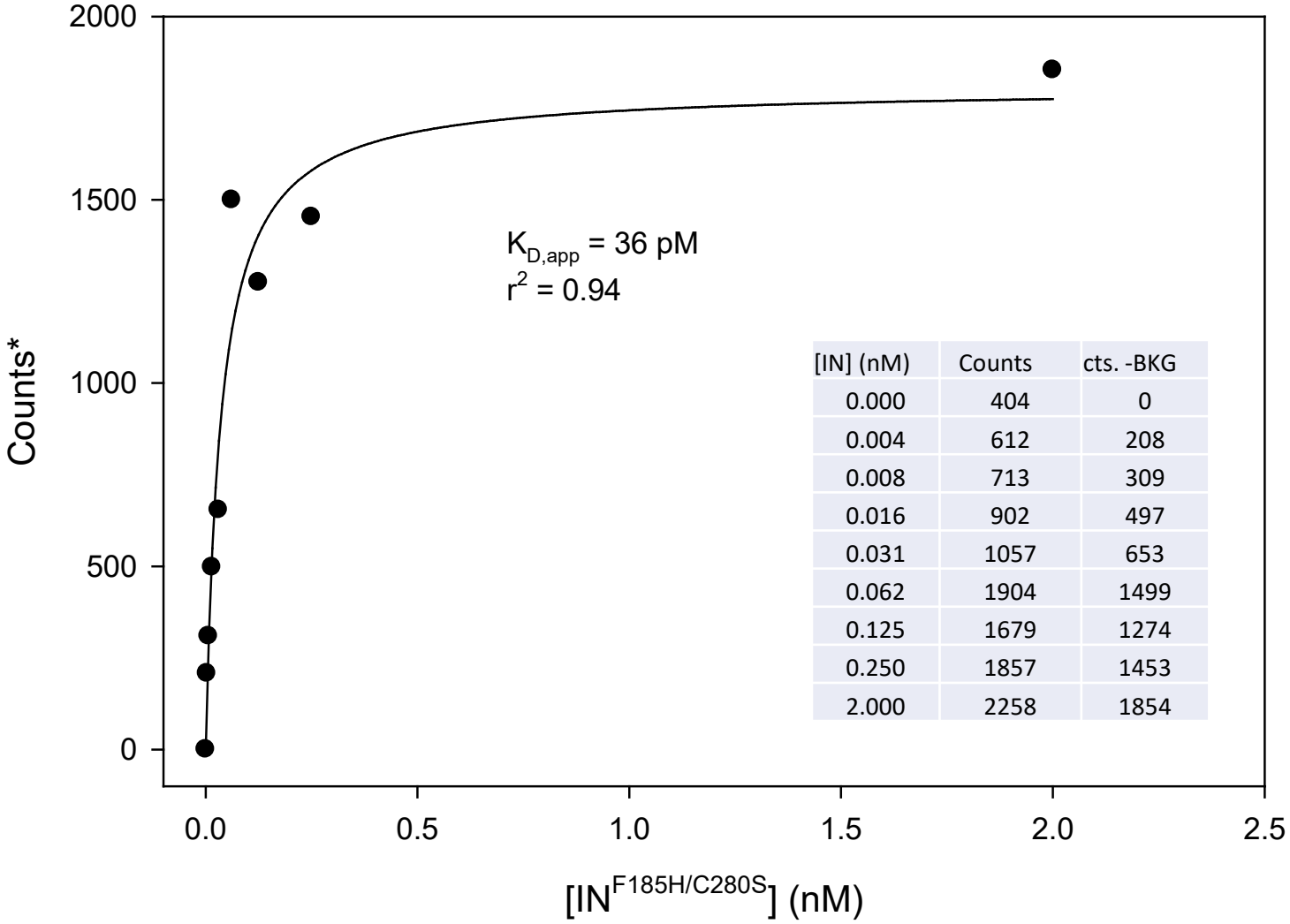

[IN] (nM)	Counts	cts. -BKG
0.000	404	0
0.004	612	208
0.008	713	309
0.016	902	497
0.031	1057	653
0.062	1904	1499
0.125	1679	1274
0.250	1857	1453
2.000	2258	1854

Figure S1. Example of apparent equilibrium dissociation constant ($K_{D,app}$) determination. Standard reactions for $K_{D,app}$ determinations were performed in 1 ml of Binding Buffer (20 mM Tris-HCl pH 7.5, 200 mM NaCl, 6 mM $MgCl_2$, and 1 mM DTT) with 0.1 mg/ml BSA and 2 pM 5′ ^{32}P end-labeled aptamer. Assays were conducted as described in the article Methods section using the nitrocellulose filter binding method for measuring binding. A plot of bound aptamer vs. IN concentration was fit to the following equation for ligand binding one-site saturation in SigmaPlot in order to determine the $K_{D,app}$: $y=B_{max}(x)/(K_D+x)$ where x is the concentration of IN and y is the amount of bound aptamer. The above graph is an assay measuring the binding of aptamer IN-1.1 to HIV $IN^{F185H/C280S}$. The determined $K_{D,app}$ value and the r^2 value for the fit are shown along with a Table of the data that was plotted. *Counts refer to radioactivity counted bound to nitrocellulose filters that were determined using a scintillation counter.

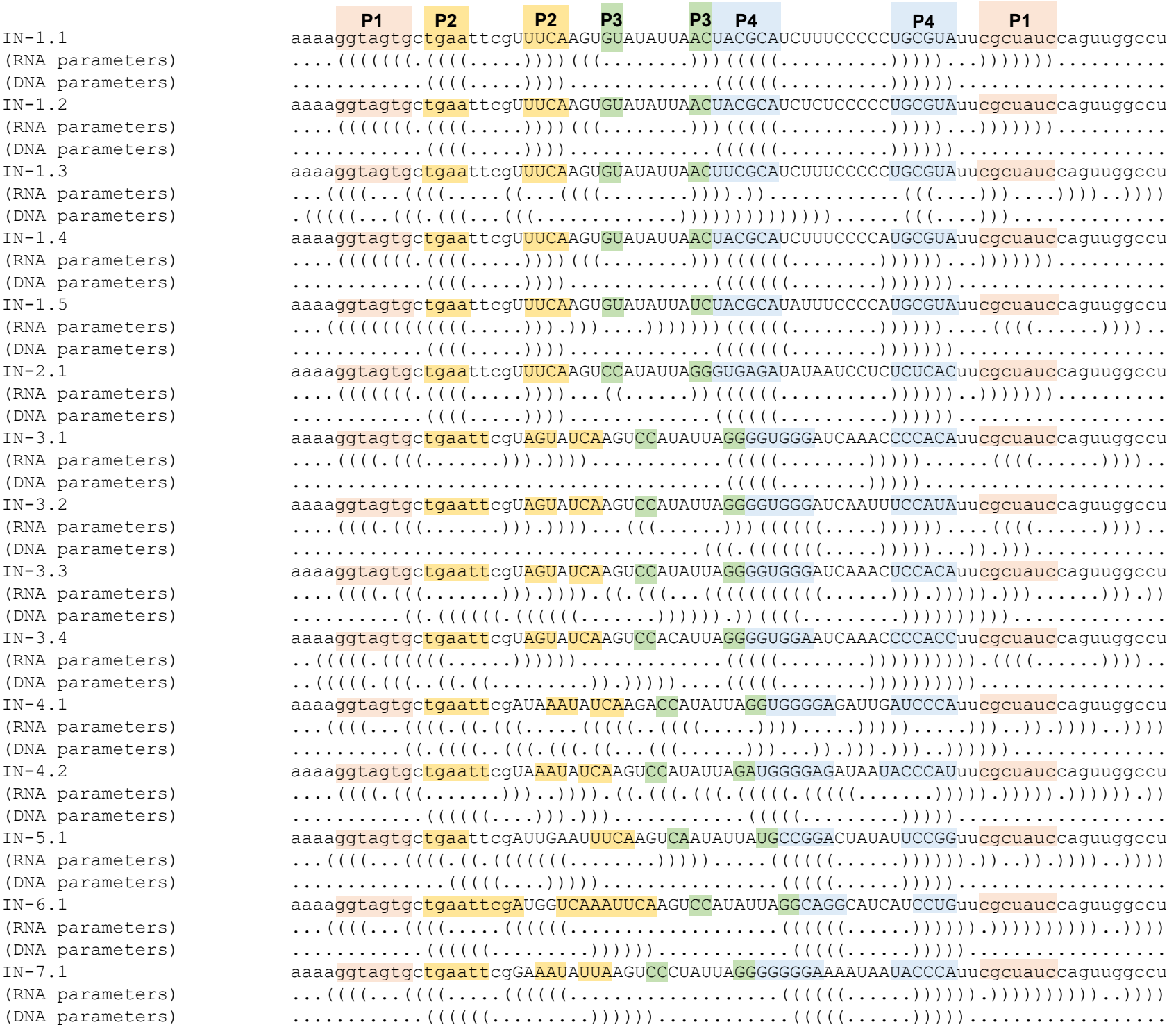

Figure S2. Predicted secondary structures of the round 10 sequences that conform to the four-way junction structural motif. All sequences from the lineages 1 – 7 are shown. The four final predicted base-pairing elements are highlighted, color coded, and labeled. Secondary structures predicted for individual sequences by RNAfold using default RNA parameters (RNA parameters) and those predicted using DNA energy parameters (DNA parameters) are shown in standard bracket notation.

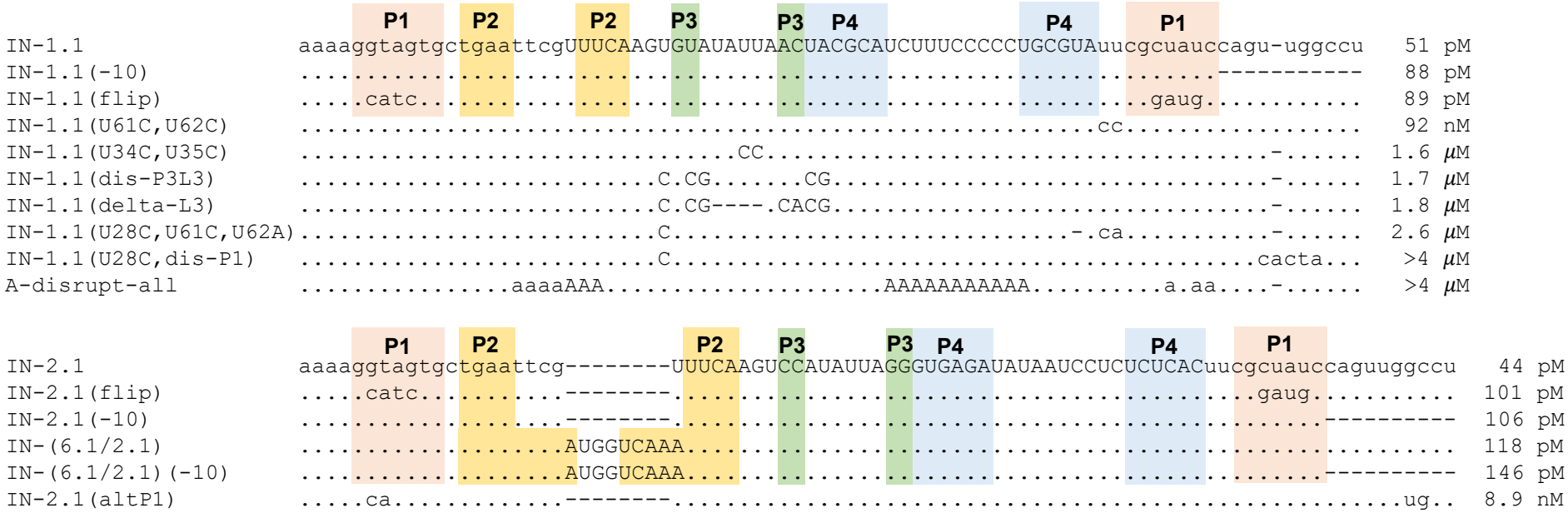

Figure S3. Sequences variants based on IN-1.1 and IN-1.2. The sequences are shown relative to IN-1.1 and IN-2.1. For, sequences predicted to adopt the secondary structure depicted in Figure 2 the base-pairing elements are highlighted, color coded, and labeled. All other sequences are predicted to adopt alternative structures. The $K_{D,App}$ for each construct is indicated to the right of the sequence.

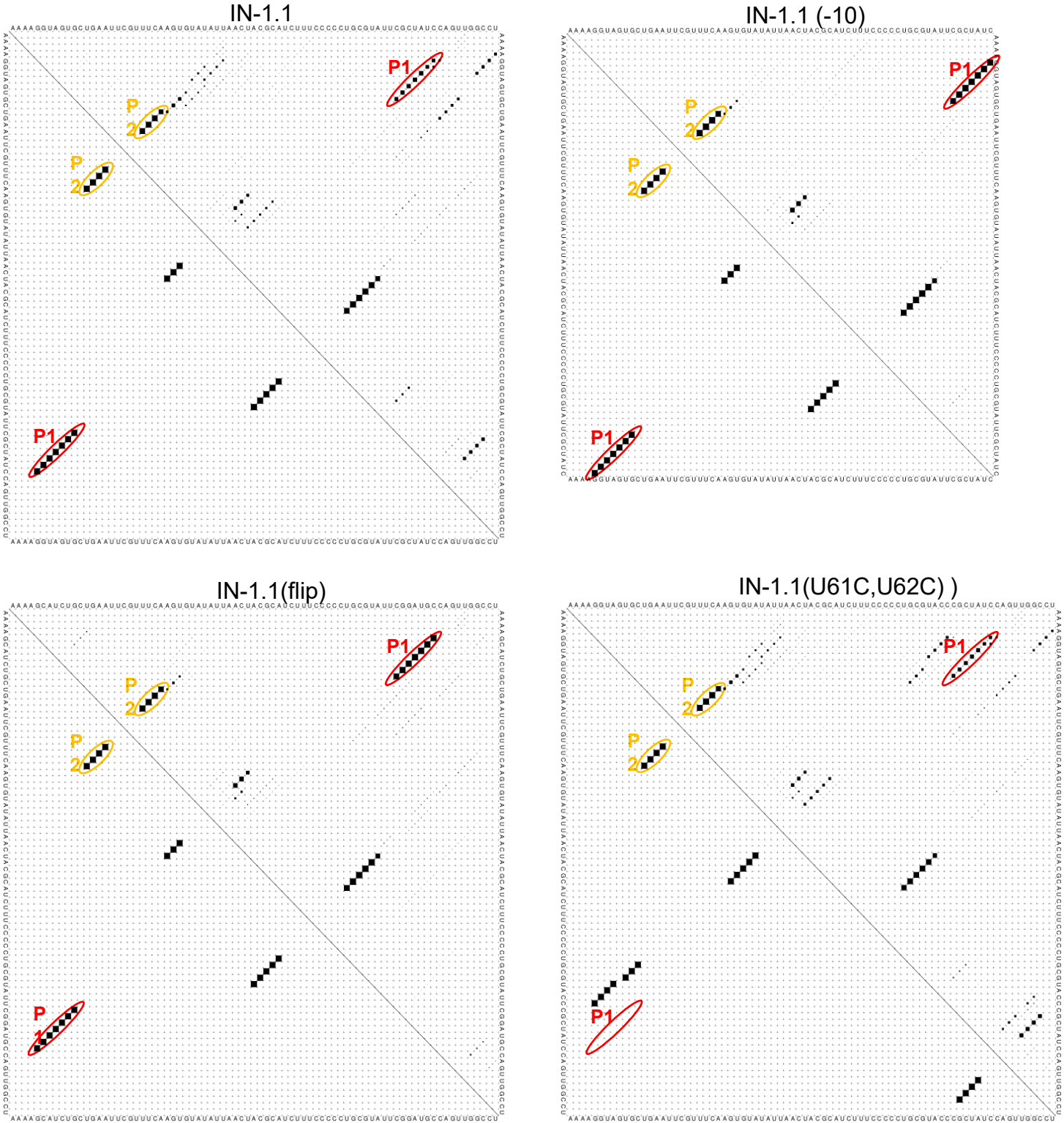

Figure S4. Predicted base-pairing probabilities for sequence variants based on IN-1.1 Dot plots containing the base-pair probabilities predicted by RNAfold are shown for the sequences indicated above the plot. The squares above the diagonal represent the base-pair probabilities. Above the diagonal the size of the squares is proportional to the probability of the base-pair. The squares below the diagonal represent the base-pairs present in the predicted minimum free energy structure. The positions in the plot that correspond to P1 and P2 are circled and labeled.

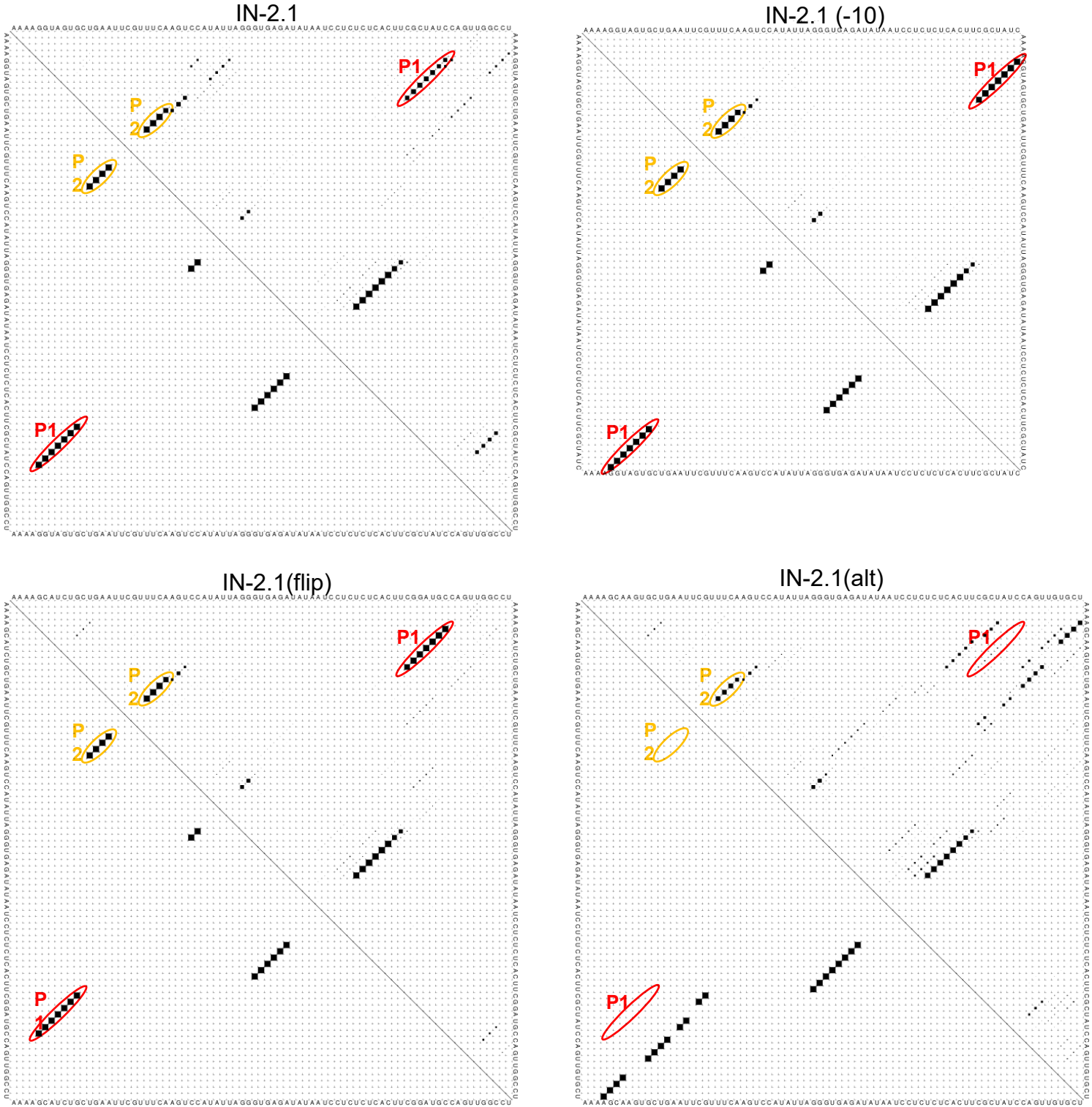

Figure S5. Predicted base-pairing probabilities for sequence variants based on IN-2.1 Dot plots containing the base-pair probabilities predicted by RNAfold are shown for the sequences indicated above the plot. The squares above the diagonal represent the base-pair probabilities. Above the diagonal the size of the squares is proportional to the probability of the base-pair. The squares below the diagonal represent the base-pairs present in the predicted minimum free energy structure. The positions in the plot that correspond to P1 and P2 are circled and labeled.