

Figure S1. RMSD plot of T30695 aptamer in the presence of Pb^{2+} at the different temperatures during 100 ns MD simulations.

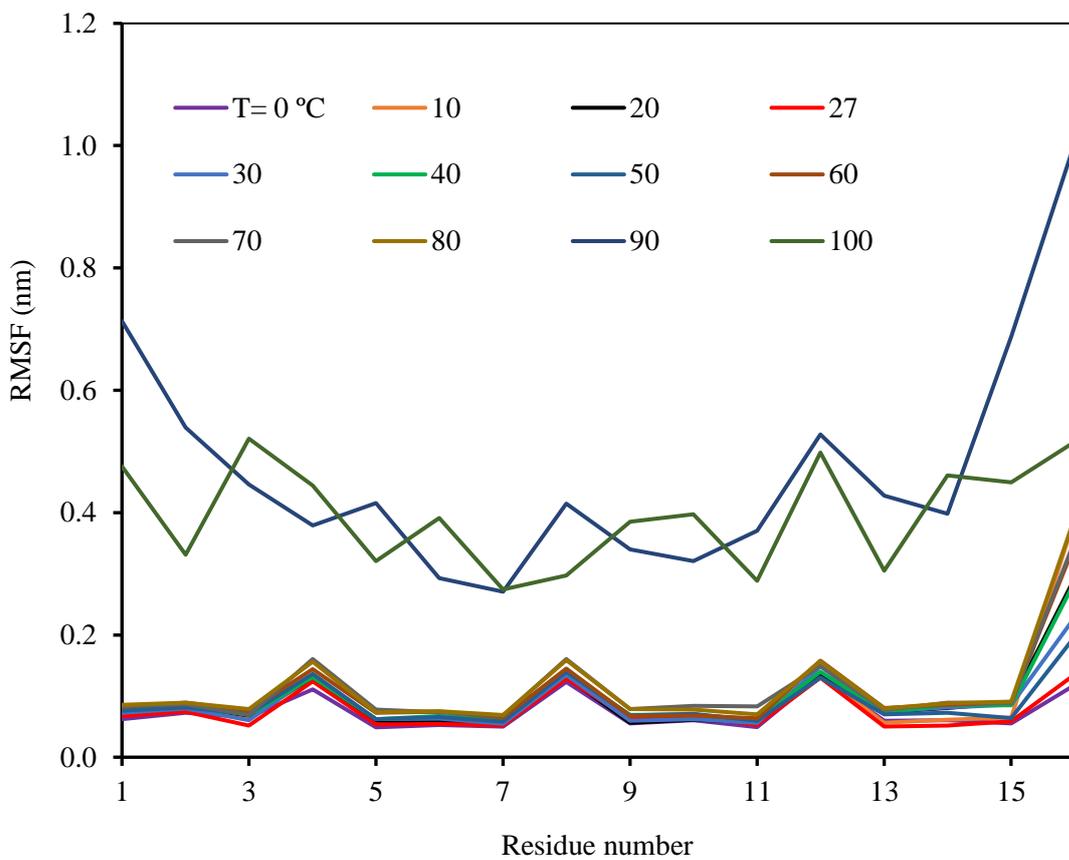


Figure S2. RMSF plot of T30695 aptamer in the presence of Pb^{2+} at the different temperatures during 100 ns MD simulations.

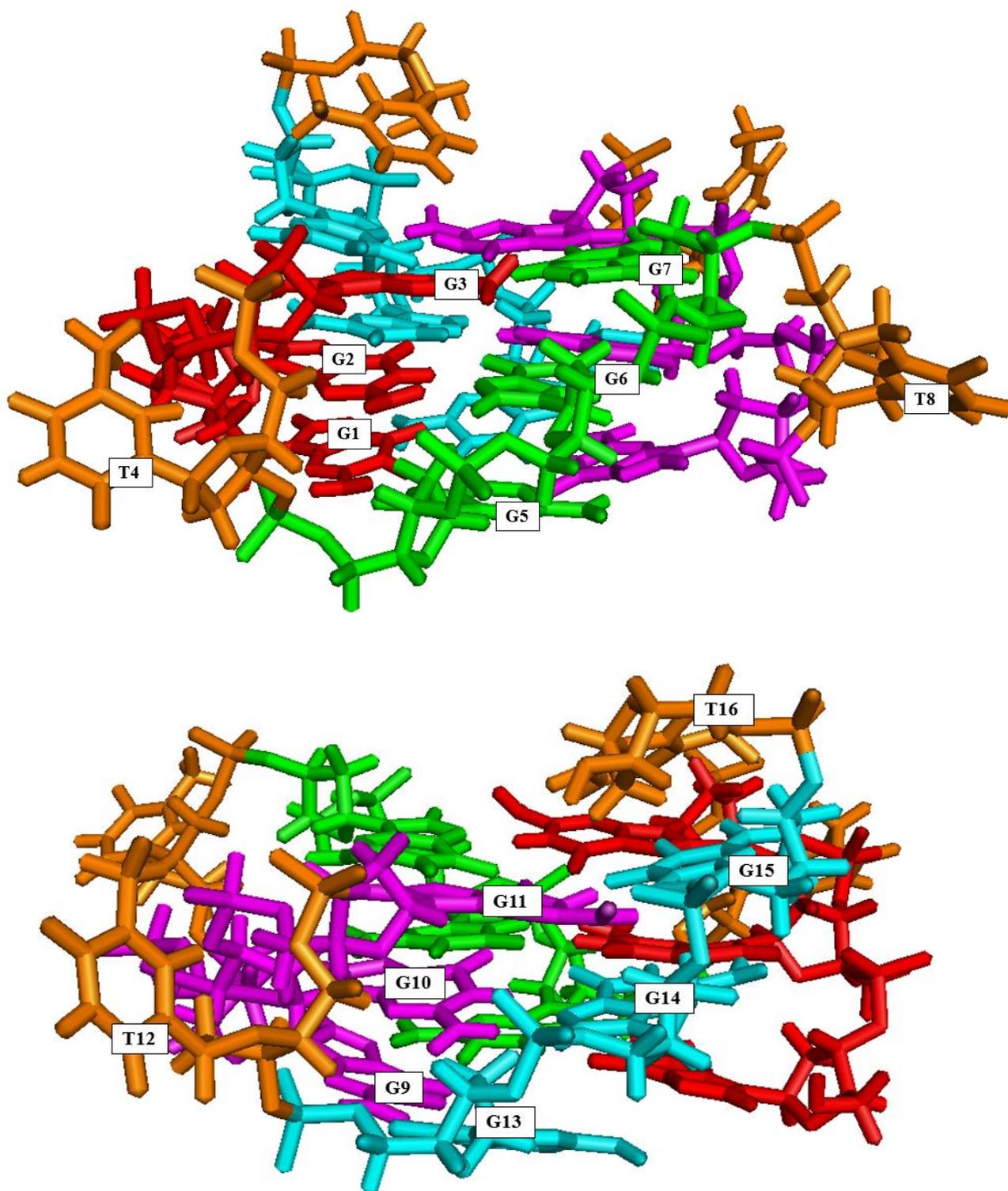


Figure S3. The type and number of the nucleotides of T30695 aptamer. Reprinted with permission [67].

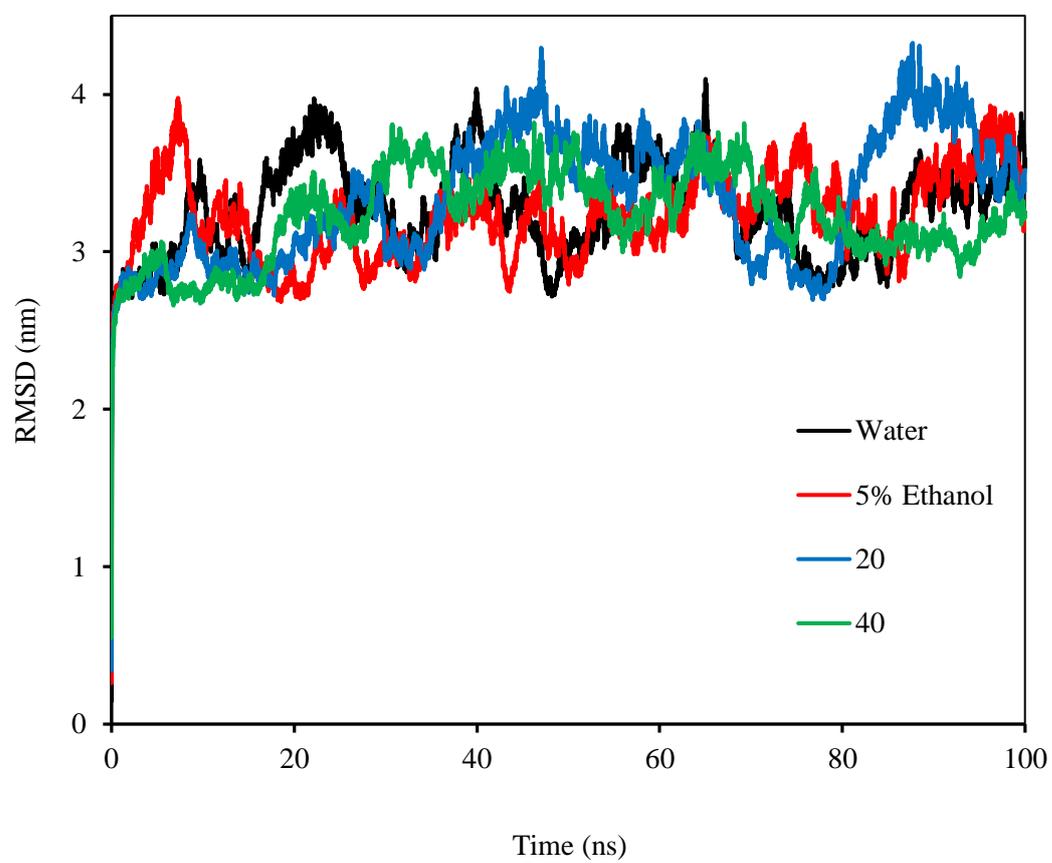


Figure S4. RMSD plot of T30695 aptamer in the presence of Pb^{2+} with the different molecular crowding conditions during 100 ns MD simulations.

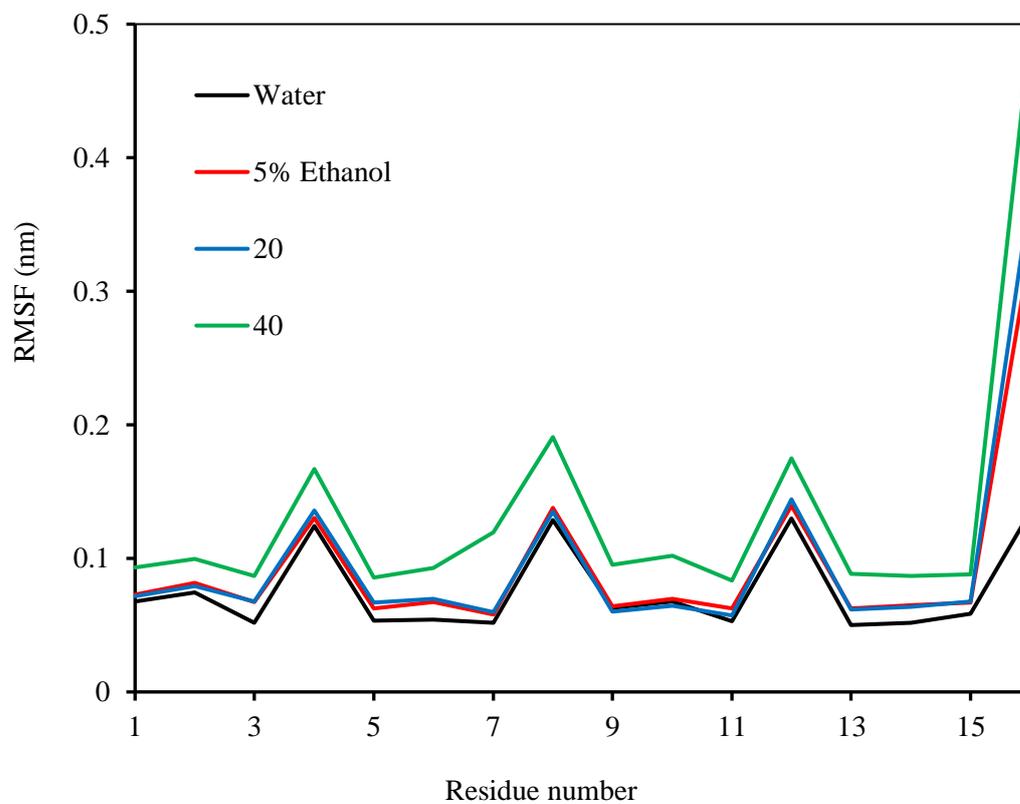


Figure S5. RMSF plot of T30695 aptamer in the presence of Pb^{2+} with the different molecular crowding conditions during 100 ns MD simulations.

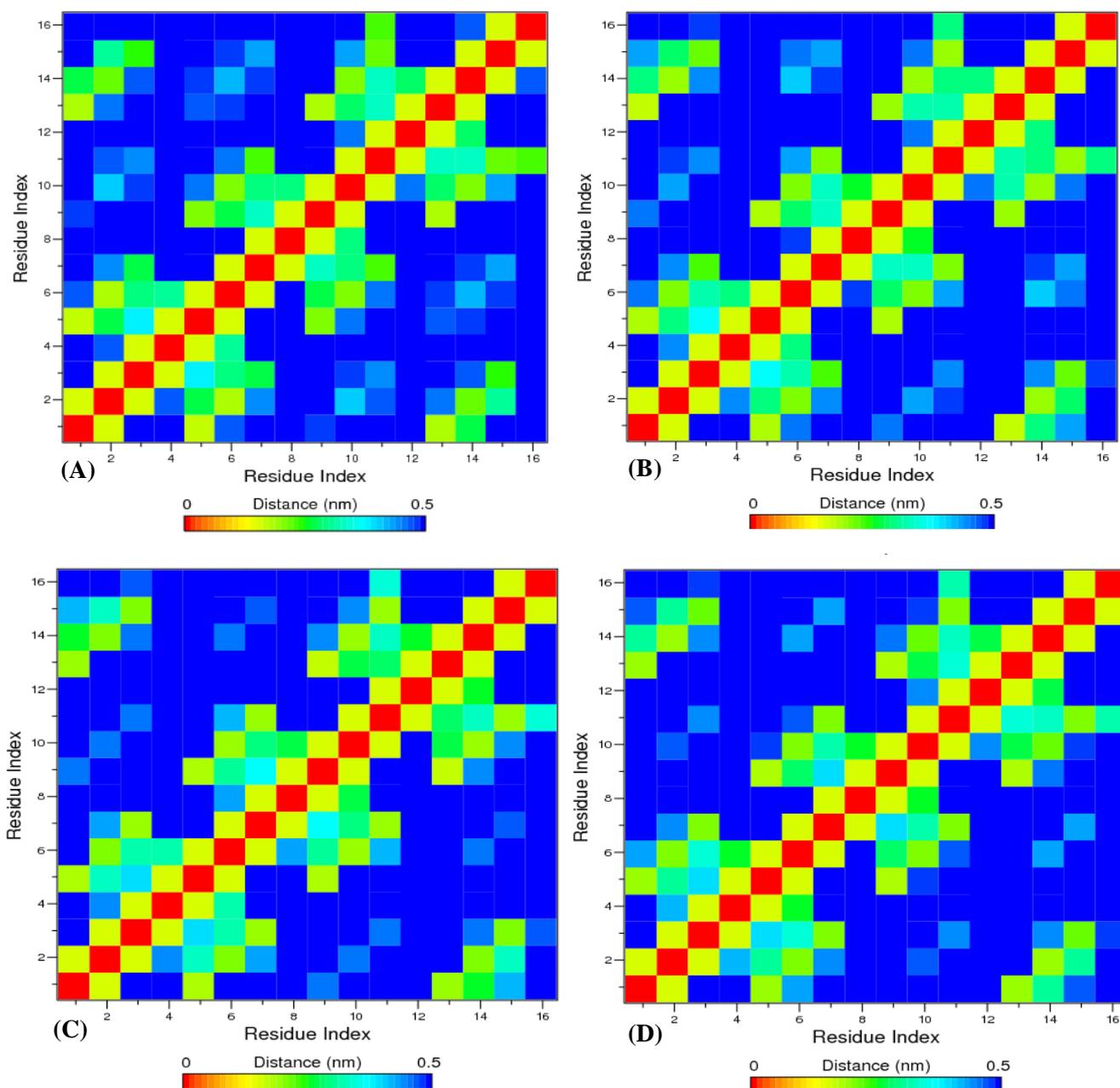


Figure S6. Contact maps of T30695 aptamer in the presence of Pb^{2+} and ethanol as the molecular crowding agent with the different concentrations, 0, 5, 20, and 40% v/v (A-D), during 100 ns MD simulations.

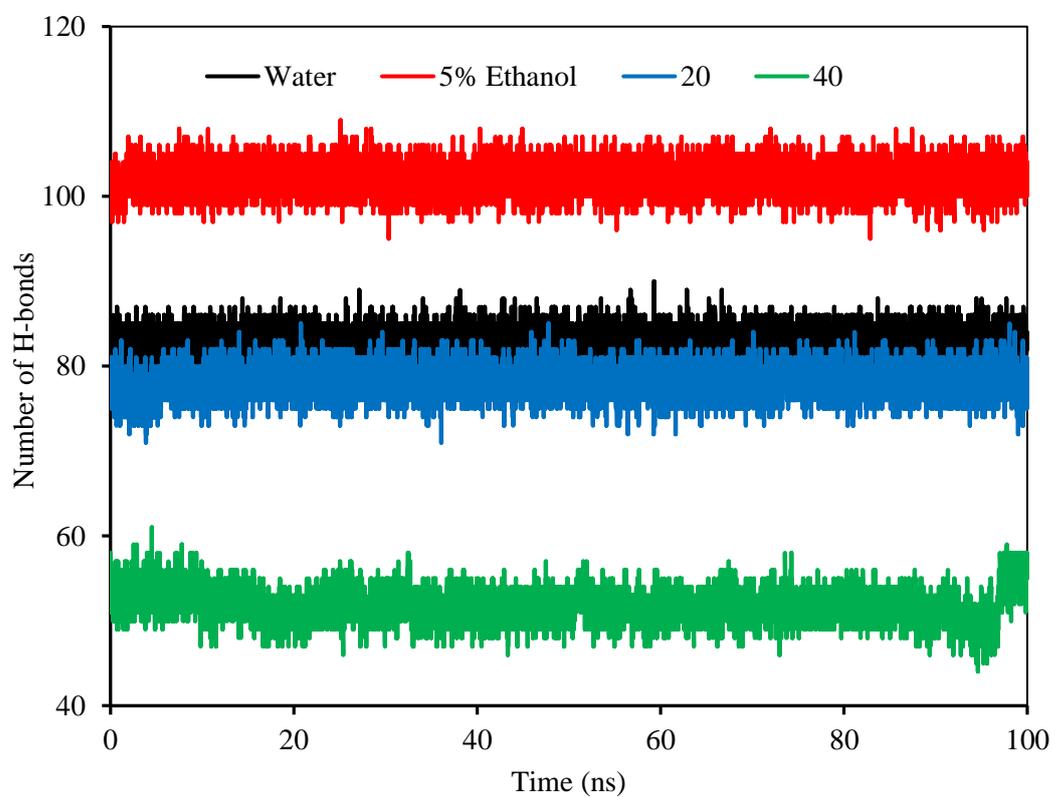


Figure S7. H-bond analysis of T30695 aptamer in the presence of Pb^{2+} with the different molecular crowding conditions during 100 ns MD simulations.

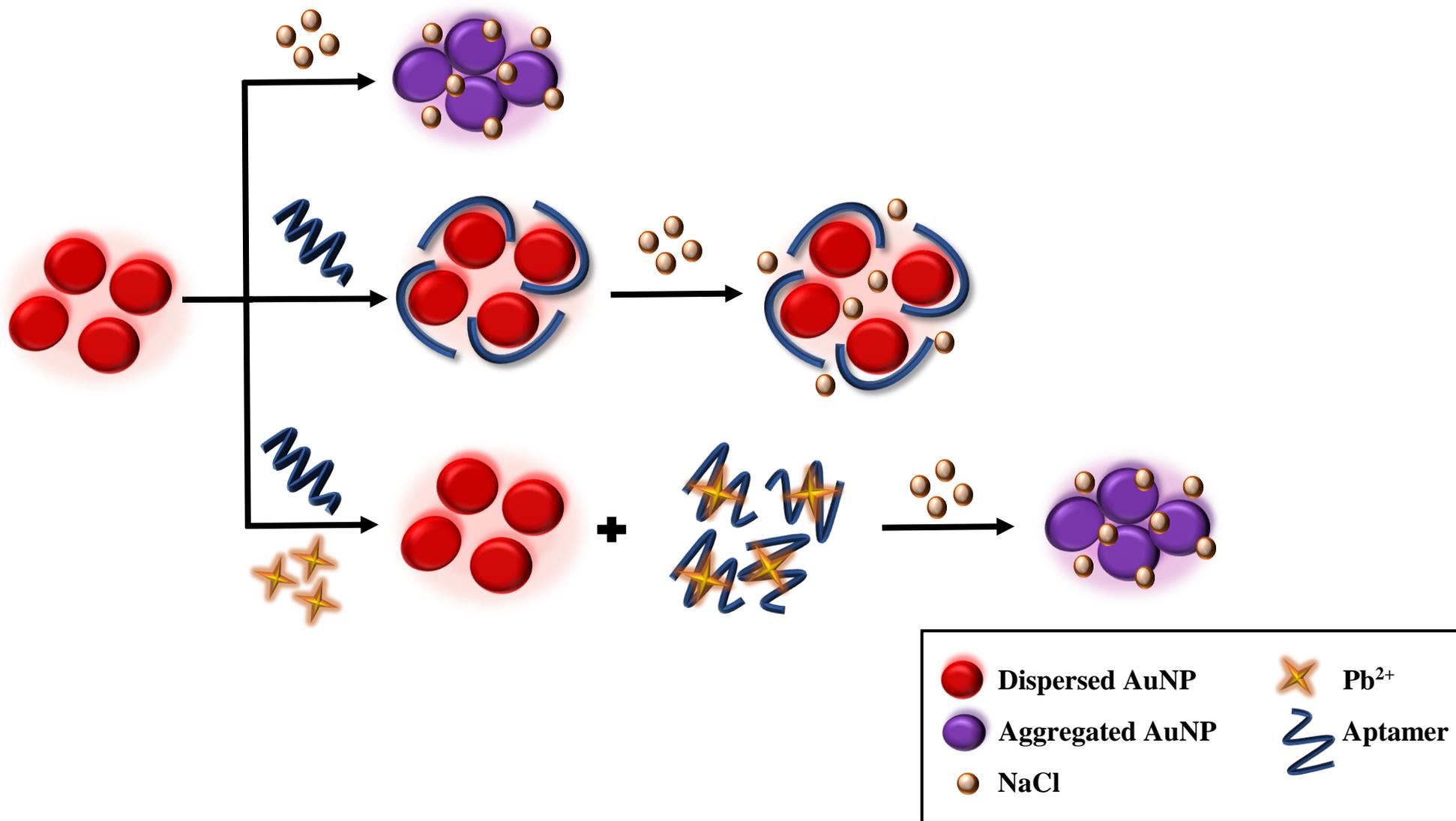


Figure S8. Schematic representation of the colorimetric assay for the Pb^{2+} detection.

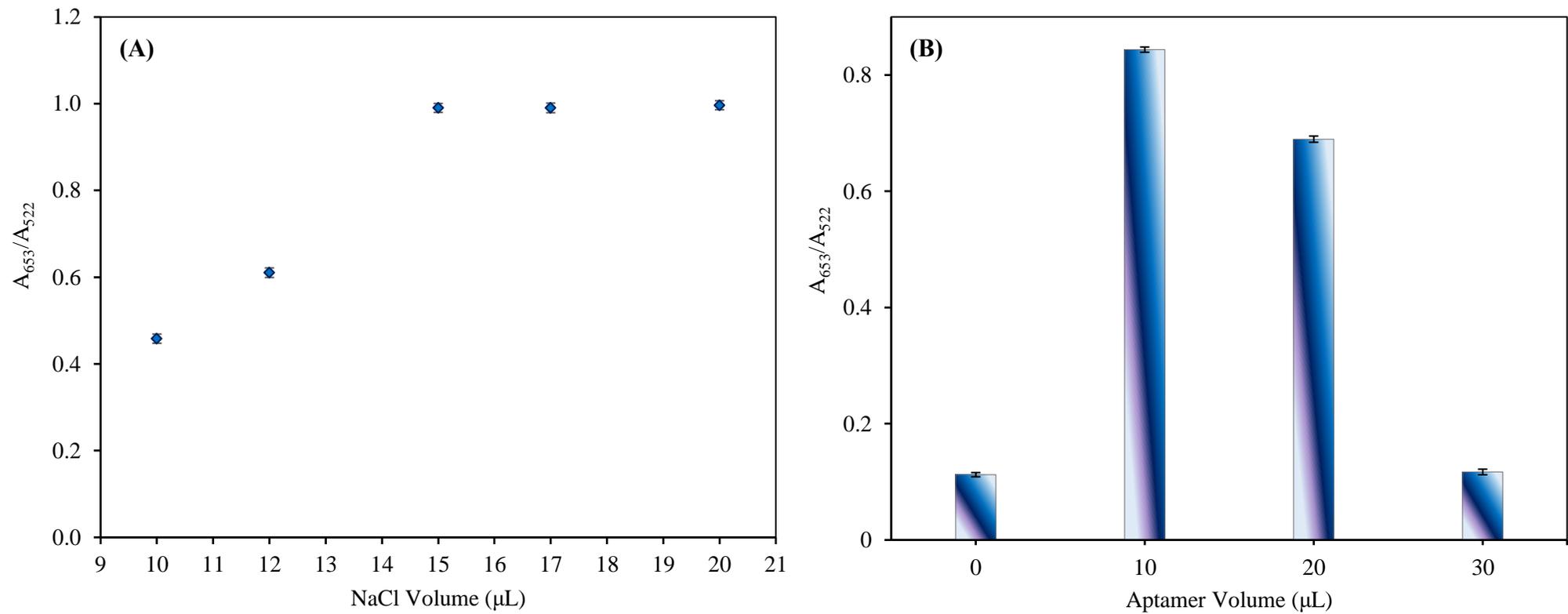


Figure S9. (A) A_{653}/A_{522} of AuNPs (100 μL) in the presence of the different volumes of NaCl (0.5 mM). (B) A_{653}/A_{522} of AuNPs in the presence of the different volumes of the aptamer solution (1 μM) after addition of the NaCl (0.5 mM, 15 μL). The error bars represent the average standard errors for three measurements.

Table S1 The contacts between the nucleotides of T30695 aptamer in the presence of ethanol as the crowding agent the different concentrations (% v/v).

Contacts	0	5	20	40
G1-G6	C	B	C	B
G1-G9	C	B	B	C
G1-G15	C	B	B	C
G2-T4	C	B	B	B
G2-G15	B	A	B	B
G3-T4	A	A	B	B
G3-T16	C	B	B	C
G5-G9	C	B	B	B
G6-G11	C	B	B	C
G6-G13	C	B	C	C
G6-T14	B	A	C	B
G6-G15	C	B	C	C
G10-T12	B	B	C	B

A: very close, B: close, and C: far (based on the index of color in Figure S6).