OMTN, Volume *25*

Supplemental information

The role of SAXS and molecular simulations in 3D structure elucidation of a DNA aptamer against lung cancer

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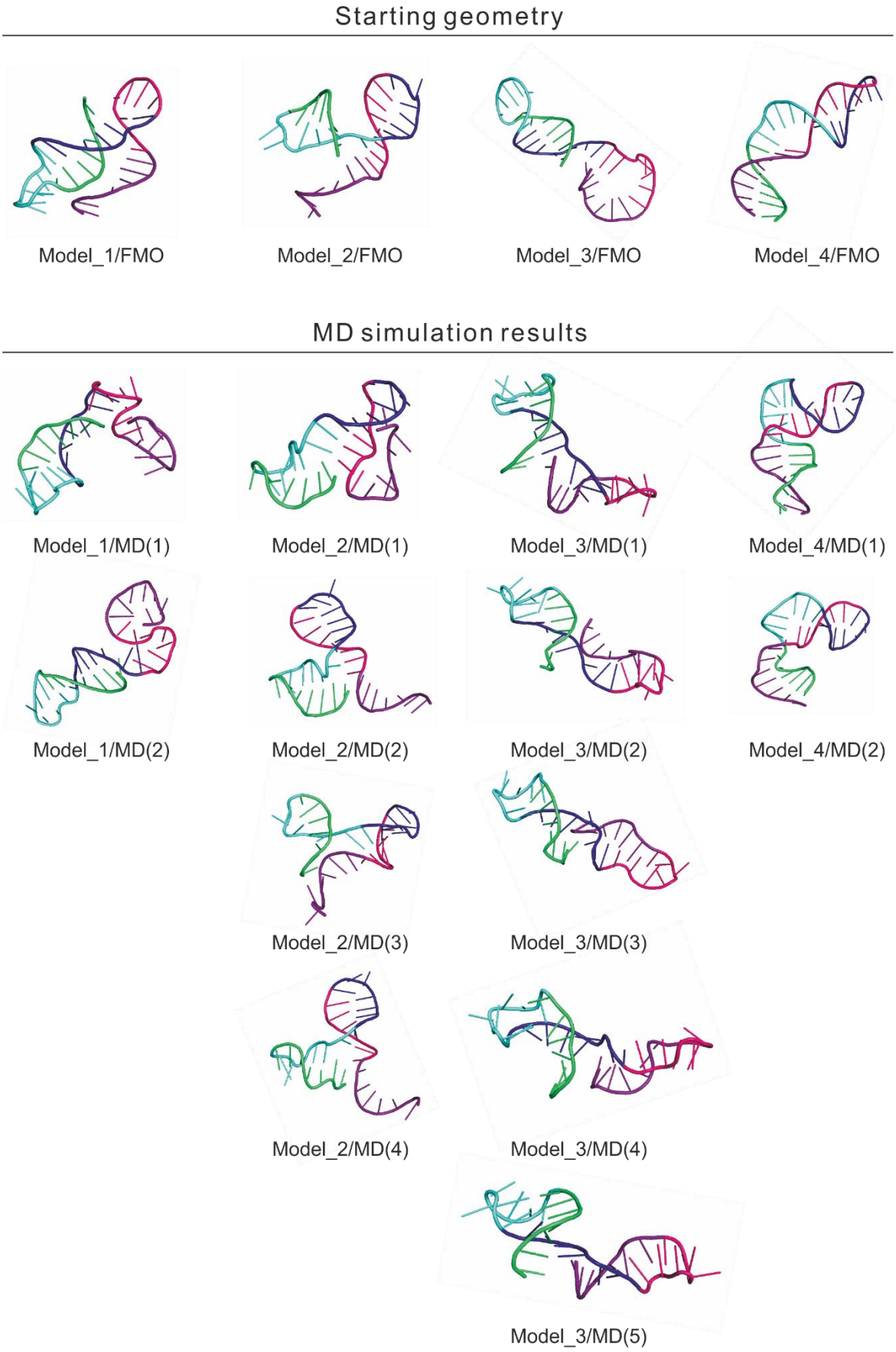

Figure S1. MD simulation results for the LC-18t aptamer. LC-18t is shown in different colors, where 5'-end is green, 3'-end is purple; the number in parentheses indicates the cluster number.

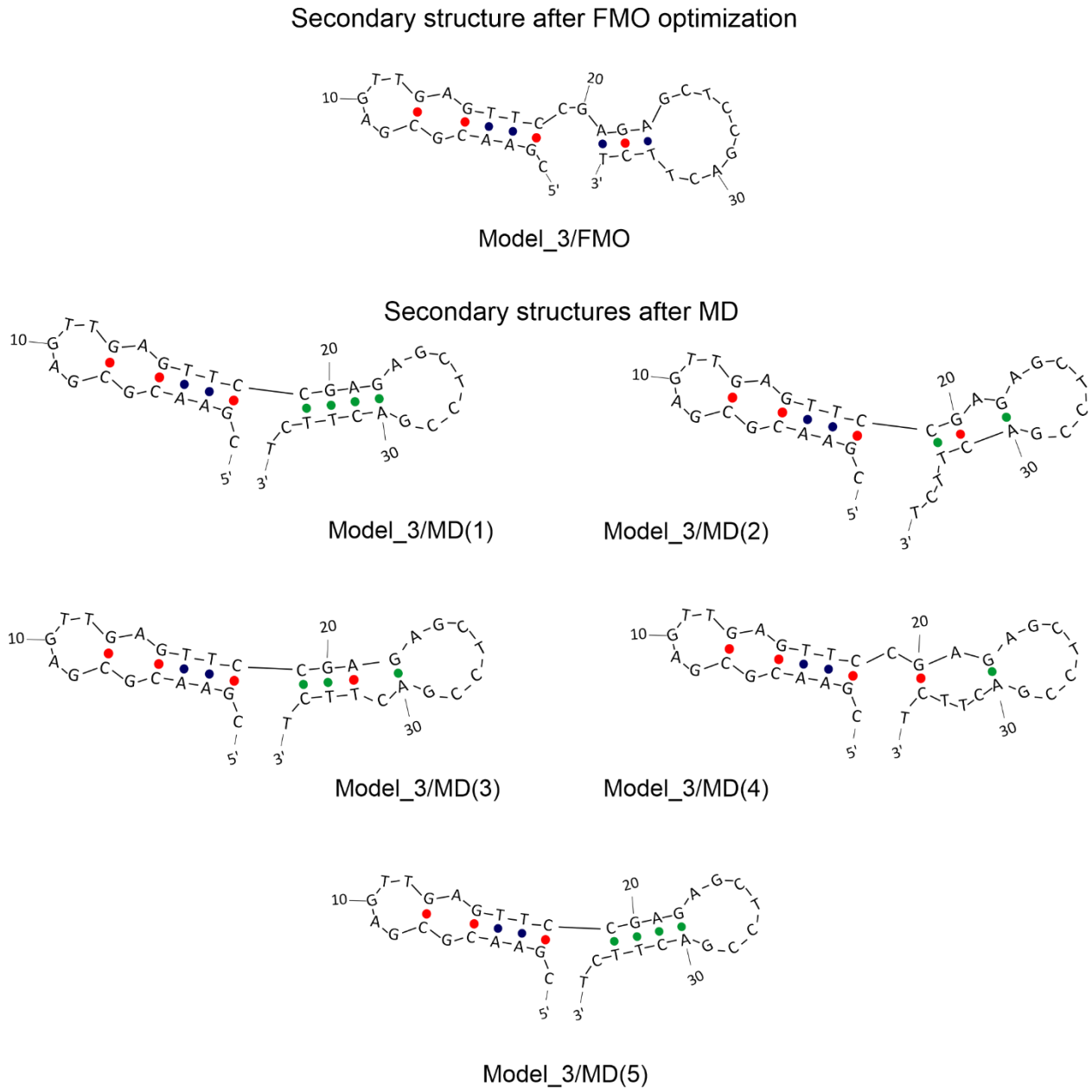

Figure S2. The secondary structure of Model3 after FMO calculations and after MD simulations.

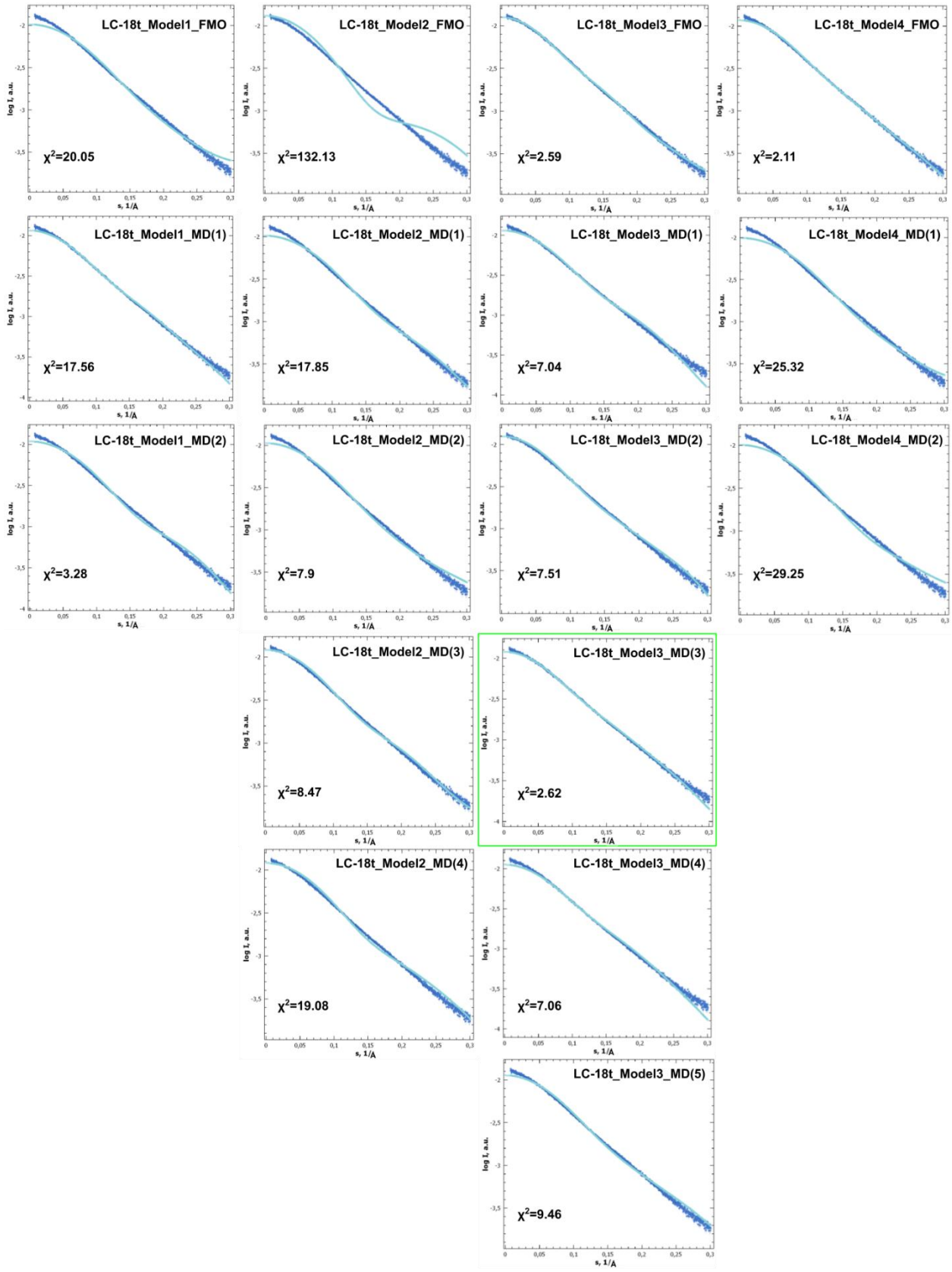

Figure S3. Comparison of the experimental SAXS and simulated scattering curves. The best model from molecular dynamics is enclosed in a green square. The values of the deviations are computed with CRYSOL program.

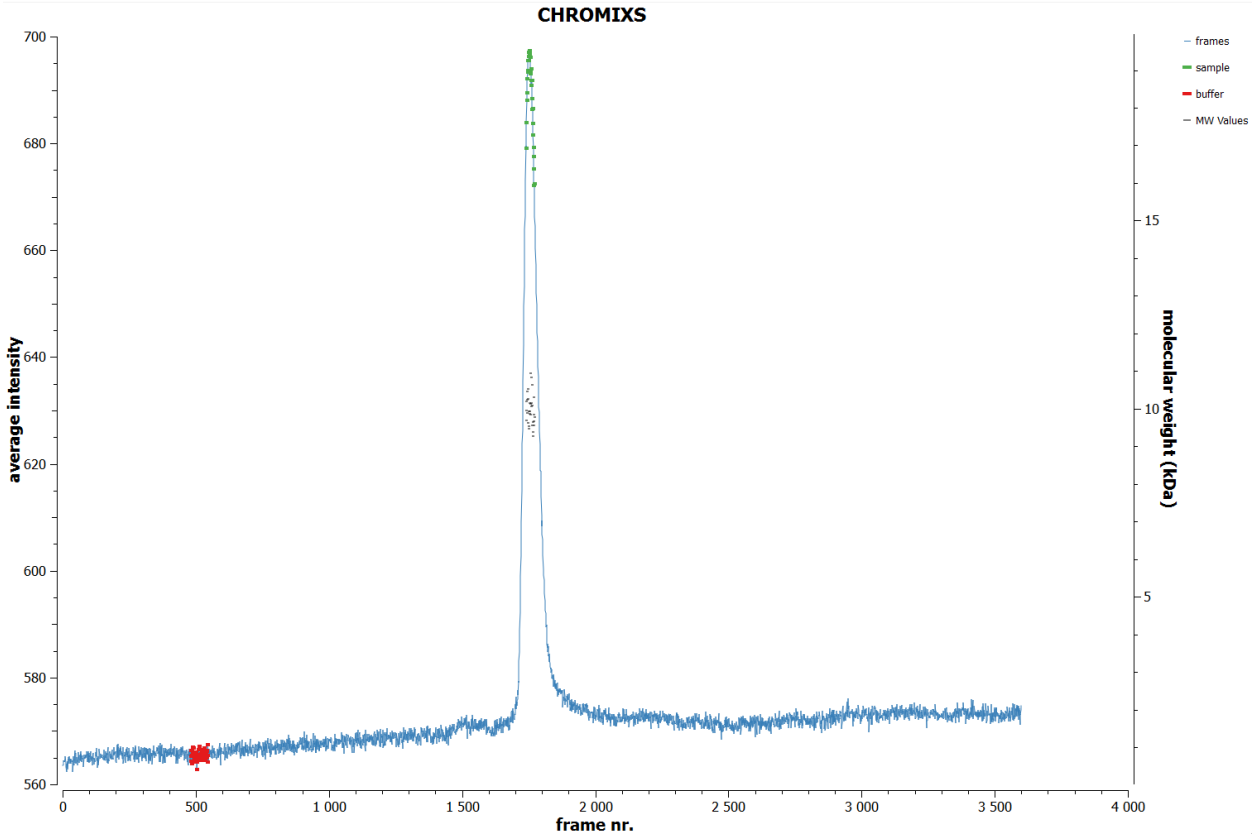

Figure S4. SEC-SAXS plot produced by CHROMIXS program. It represents the chromatogram for the LC-18t aptamer showing the monodispersity of the sample and counting 3600 SAXS measurement points. From the number of these points corresponding to the peak of UV absorbance and therefore maximum concentration of the sample in the solution one can estimate the molecular weight and the radius of gyration.

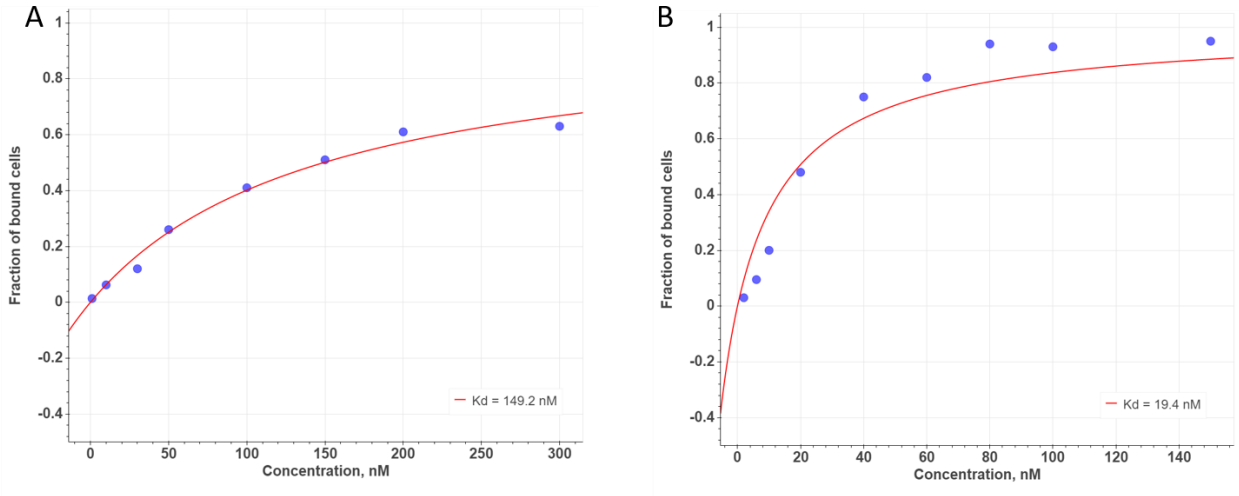

Figure S5. Determination of binding affinity to lung cancer cells, Kd value of the DNA-aptamers LC-18 (A) or LC-18t (B) by flow cytometry. The percentage of bound LC cells measured in the Direct coordinates.

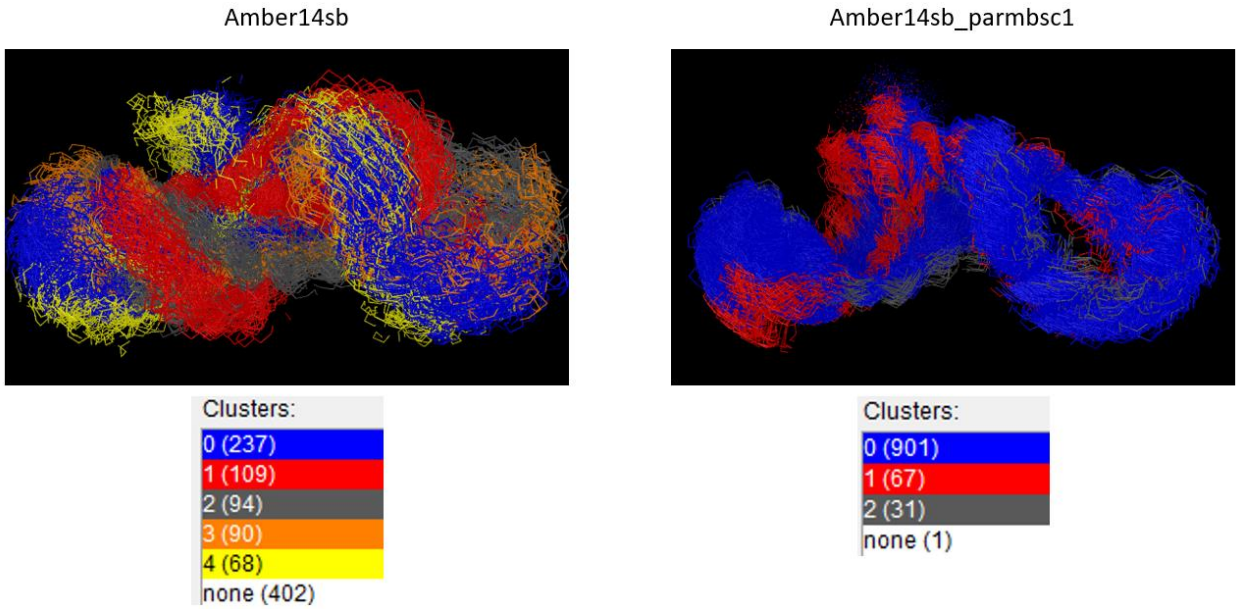

Figure S6. Comparison of LC-18t aptamer simulation (Model3) between Amber14sb (left panel) and Amber14sb_parmbsc1 (right panel) force fields. Clusterization has been performed in VMD using RMSD of the Phosphorus atoms with a threshold of 0.4 nm (see the main text for the full clusterization protocol). One could note that the regular Amber14sb force field shows a much better sampling of the conformational space of the aptamer than the parmbsc1 variant. We could speculate here that the parmbsc1 forcefield, in general, keeps better DNA duplex form; however, for aptamers, this could lead to much less flexibility.