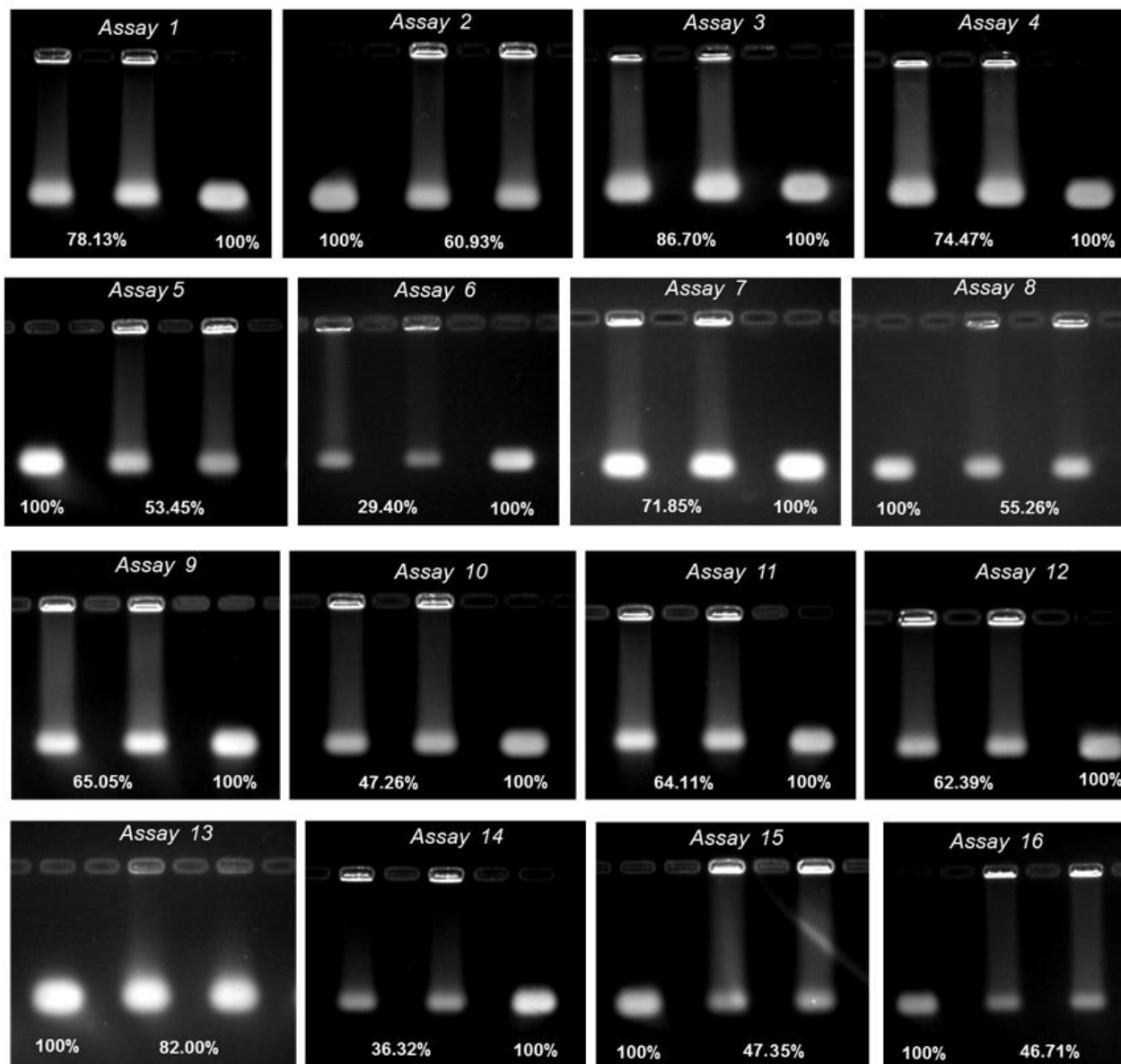


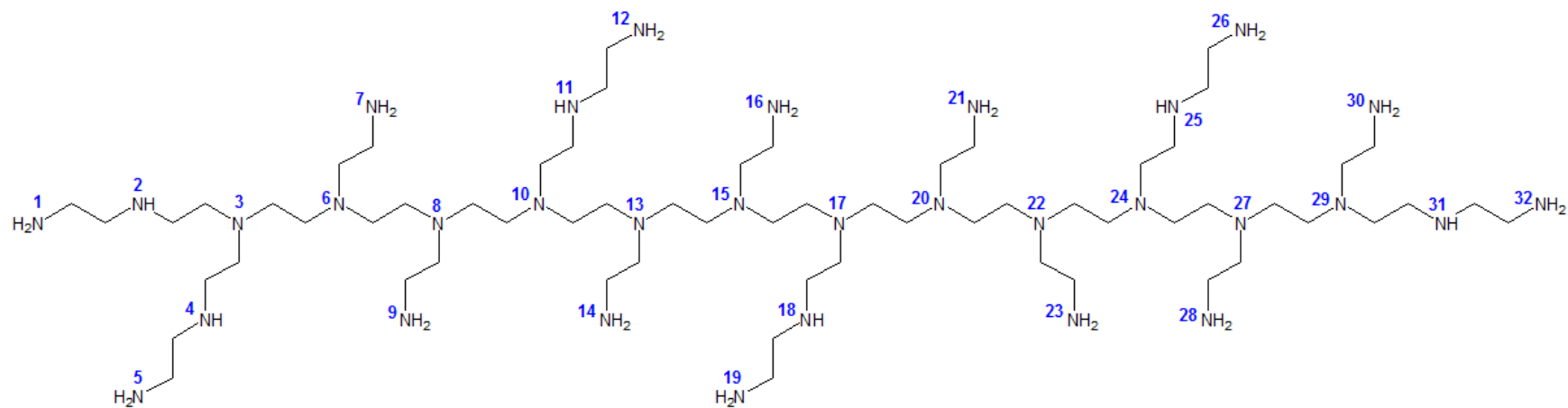
**ELECTRONIC SUPPLEMENTARY INFORMATION**

**Experimental design, modeling and optimization of polyplex formation  
between DNA oligonucleotide and branched polyethylenimine**

Lilia Clima, Elena L. Ursu, Corneliu Cojocaru, Alexandru Rotaru\*, Mihail Barboiu  
and Mariana Pinteala

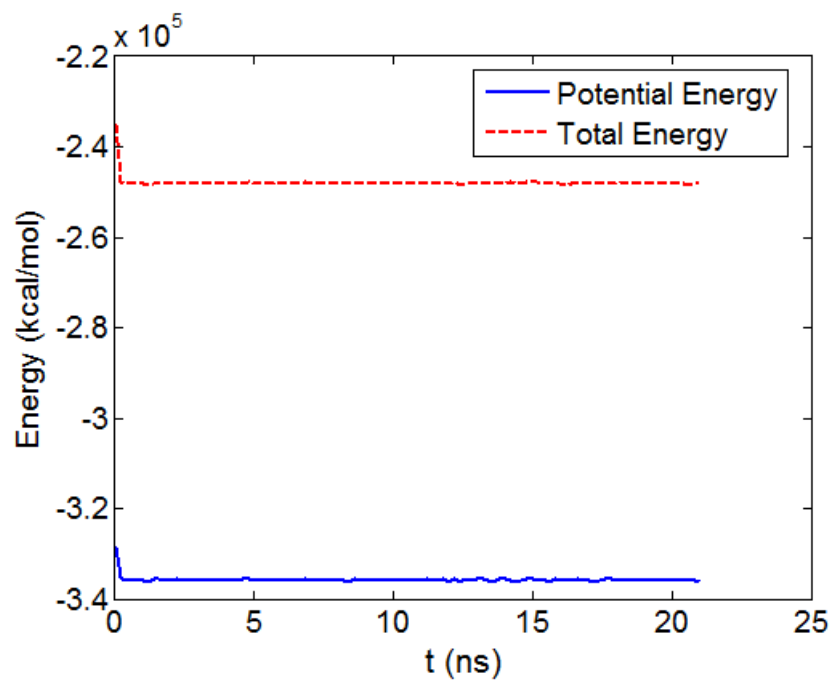


**Fig. S1.** Gel electrophoresis assays performed according to the designed conditions from Table 2, containing a reference band (100%) and the average values for unbound dsDNA bands.

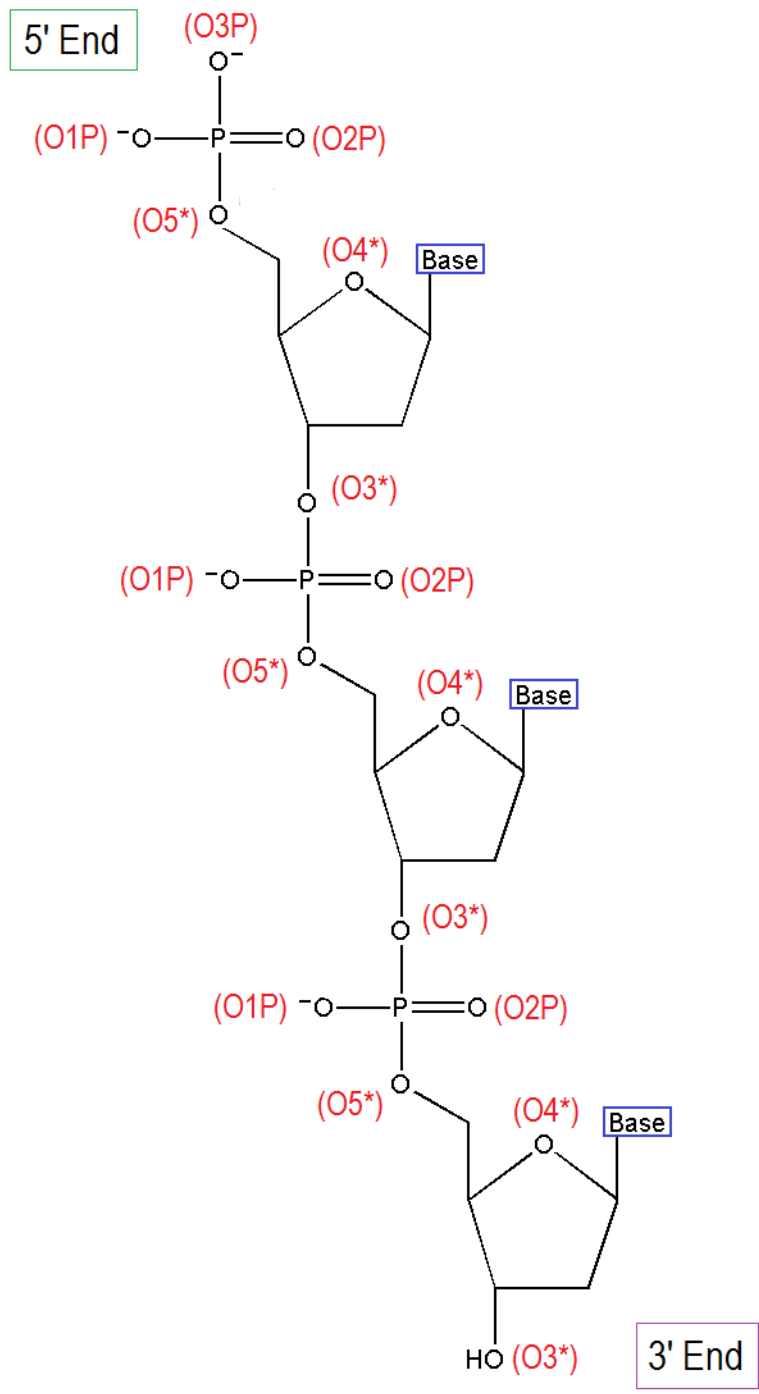


**Fig. S2.** Scheme of molecular structure of branched-polyethylenimine (B-PEI) with nitrogen numbering

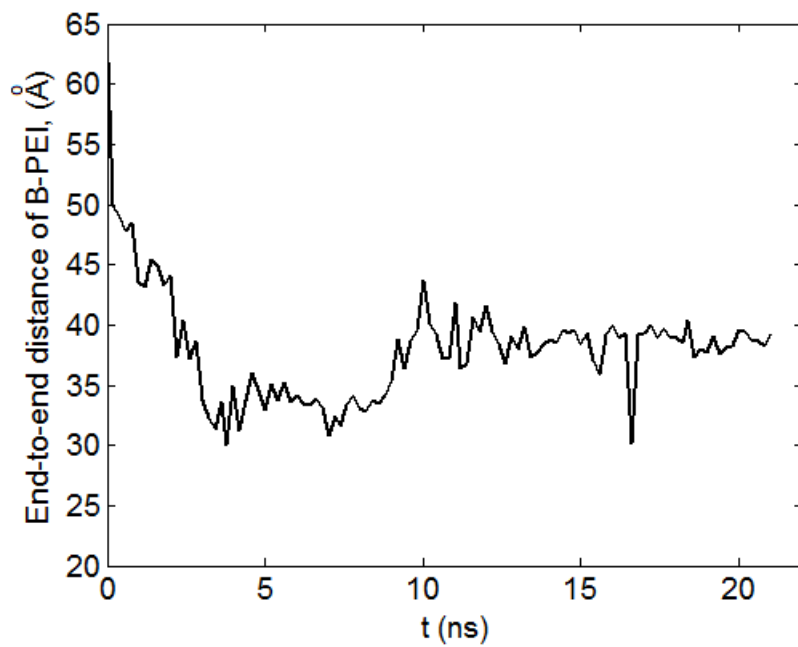
(indexed by numbers near nitrogen atoms).



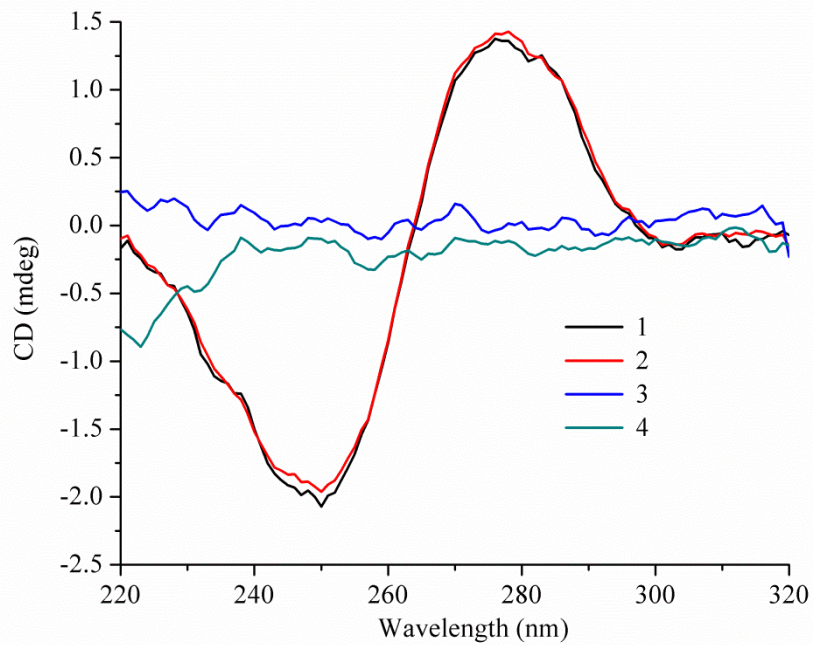
**Fig. S3.** Potential and total energy of the molecular system (dsDNA / B-PEI / Water) against the simulation time.



**Fig. S4.** Notations and positions of DNA backbone oxygen atoms, (O1P, O2P, O3P, O3\*, O4\* and O5\*).



**Fig. S5.** Interatomic 1N-32N distance for B-PEI (end-to-end distance) versus simulation time.



**Fig. S6. Circular Dichroism analysis of samples with D/P ratio of 1.144 at pH=5.8.**

1. dsDNA: 1.51  $\mu\text{M}$  ds DNA, 10.8 mM TRIS, 5.4mM acetic acid, 270  $\mu\text{M}$  EDTA, 7.5 $\mu\text{M}$  NaCl;
2. dsDNA-B-PEI: 1.51  $\mu\text{M}$  ds DNA, 1.324  $\mu\text{M}$  B-PEI, 10.8 mM TRIS, 5.4 mM acetic acid, 270  $\mu\text{M}$  EDTA, 7.5 $\mu\text{M}$  NaCl;
3. Buffer: 10.8 mM TRIS, 5.4mM acetic acid, 270  $\mu\text{M}$  EDTA;
4. B-PEI: 1.324  $\mu\text{M}$  B-PEI, 10.8 mM TRIS, 5.4mM acetic acid, 270  $\mu\text{M}$  EDTA.