

S1 Table. Details of each simulation performed in this work with relative ID in the BigNASim database.

| Single duplex | | | | | | |
|--|---------|---------------|-----------|--------|----------|-----------------------------|
| Duplex | Cation | Concentration | Time | #H2O | #Cations | ID |
| AT-rich | Na | 25 mM | 400 ns | 19352 | 47 | AT-rich_Na_25mM |
| AT-rich | Lys | 25 mM | 400 ns | 19299 | 9 | AT-rich_Lys_25mM |
| AT-rich | Arg | 25 mM | 400 ns | 19286 | 9 | AT-rich_Arg_25mM |
| AT-rich | Orn | 25 mM | 400 ns | | 9 | AT-rich_Orn_25mM |
| AT-rich | DABA | 25 mM | 400 ns | | 9 | AT-rich_DABA_25mM |
| GC-rich | Na | 25 mM | 400 ns | 19359 | 47 | GC-rich_Na_25mM |
| GC-rich | Lys | 25 mM | 400 ns | 19313 | 9 | GC-rich_Lys_25mM |
| GC-rich | Arg | 25 mM | 400 ns | 19295 | 9 | GC-rich_Arg_25mM |
| GC-rich | Orn | 25 mM | 400 ns | | 9 | GC-rich_Orn_25mM |
| GC-rich | DABA | 25 mM | 400 ns | | 9 | GC-rich_DABA_25mM |
| AT-rich | Na | 500 mM | 400 ns | 19016 | 215 | AT-rich_Na_500mM |
| AT-rich | Lys | 500 mM | 400 ns | 17765 | 177 | AT-rich_Lys_500mM |
| AT-rich | Arg | 500 mM | 400 ns | 17582 | 177 | AT-rich_Arg_500mM |
| AT-rich | Orn | 500 mM | 400 ns | | 177 | AT-rich_Orn_500mM |
| AT-rich | DABA | 500 mM | 400 ns | | 177 | AT-rich_DABA_500mM |
| GC-rich | Na | 500 mM | 400 ns | 19023 | 215 | GC-rich_Na_500mM |
| GC-rich | Lys | 500 mM | 400 ns | 17755 | 177 | GC-rich_Lys_500mM |
| GC-rich | Arg | 500 mM | 400 ns | 17541 | 177 | GC-rich_Arg_500mM |
| GC-rich | Orn | 500 mM | 400 ns | | 177 | GC-rich_Orn_50mM |
| GC-rich | DABA | 500 mM | 400 ns | | 177 | GC-rich_DABA_500mM |
| AT-rich | Na | 1500 mM | 400 ns | 18310 | 568 | AT-rich_Na_1500mM |
| AT-rich | Lys | 1500 mM | 400 ns | 14431 | 530 | AT-rich_Lys_1500mM |
| AT-rich | Arg | 1500 mM | 400 ns | 13777 | 530 | AT-rich_Arg_1500mM |
| AT-rich | Orn | 1500 mM | 400 ns | | 530 | AT-rich_Orn_1500mM |
| AT-rich | DABA | 1500 mM | 400 ns | | 530 | AT-rich_DABA_1500mM |
| GC-rich | Na | 1500 mM | 400 ns | 18317 | 568 | GC-rich_Na_1500mM |
| GC-rich | Lys | 1500 mM | 400 ns | 14421 | 530 | GC-rich_Lys_1500mM |
| GC-rich | Arg | 1500 mM | 400 ns | 13819 | 530 | GC-rich_Arg_1500mM |
| GC-rich | Orn | 1500 mM | 400 ns | | 530 | GC-rich_Orn_1500mM |
| GC-rich | DABA | 1500 mM | 400 ns | | 530 | GC-rich_DABA_1500mM |
| 15 duplexes - condensation assay MD (with CUFIX) | | | | | | |
| AT-rich | Neutral | 500 mM | 5 μ s | 125229 | 330 (Na) | AT-rich_crowd_neut_500mM |
| AT-rich | Na | 500 mM | 5 μ s | 123605 | 1142 | AT-rich_crowd_Na_500mM |
| AT-rich | Lys | 500 mM | 5 μ s | 114861 | 1142 | AT-rich_crowd_Lys_500mM |
| AT-rich | Arg | 500 mM | 5 μ s | 113646 | 1142 | AT-rich_crowd_Arg_500mM |
| GC-rich | Neutral | 500 mM | 5 μ s | 125202 | 330 (Na) | GC-rich_crowd_neut_500mM |
| GC-rich | Na | 500 mM | 5 μ s | 123578 | 1142 | GC-rich_crowd_neut_Na_500mM |
| GC-rich | Lys | 500 mM | 5 μ s | 115011 | 1142 | GC-rich_crowd_Lys_500mM |
| GC-rich | Arg | 500 mM | 5 μ s | 113692 | 1142 | GC-rich_crowd_Arg_500mM |