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Supplemental Information

Ensembles of Breathing Nucleosomes: A Computational Study

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Ensembles of breathing nucleosomes: a computational study

Supplemental Material

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|---------------|-------------|------------|------------|------------|
| 601 | CTGGAGAATC | CCGGTGCCGA | GGCCGCTCAA | TTGGTCGTAG |
| | ACAGCTCTAG | CACCGCTTAA | ACGCACGTAC | GCGCTGTCCC |
| | CCGCGTTTTA | ACCGCAAGG | GGATTACTCC | CTAGTCTCCA |
| | GGCACGTGTC | AGATATATAC | ATCCTGT | |
| 601RTA | CTGGAGAATC | CCGGTGCCGA | GGCCGCTCAA | TTGGTCGTAG |
| | ACAGCTCTAG | CACCGCTTAA | ACGCACGTAC | GCGCTGTCTA |
| | CCGCGTTTTA | ACCGCAATA | GGATTACTTA | CTAGTCTCCA |
| | GGCACGTGTC | AGATATATAC | ATCCTGT | |
| 601MF | CTGGAGAATC | CCGGTGCCGA | GGCCGCTCAA | TTGGTCGGA |
| | GTAATCCCT | TGGCGGTAA | AACGCGGGG | ACACCGCGTA |
| | CGTGCGTTA | AGCGGTGCTA | GAGCTGTCTA | CTAGTCTCCA |
| | GGCACGTGTC | AGATATATAC | ATCCTGT | |
| 601L | CTGGAGAATC | CCGGTGCCGA | GGCCGCTCAA | TTGGTCGTAG |
| | ACAGCTCTAG | CACCGCTTAA | ACGCACGTAC | GCGCCGCGTA |
| | CGTGCGTTA | AGCGGTGCTA | GAGCTGTCTA | CGACCAATTG |
| | AGCGGCTCG | GCACCGGGAT | TCTCCAG | |
| 5S | CTTCCAGGGA | TTTATAAGCC | GATGACGTCA | TAACATCCCT |
| | GACCCTTTAA | ATAGCTTAA | TTTCATCAAG | CAAGAGCCTA |
| | CGACCATAACC | ATGCTGAATA | TACCGTTCT | CGTCCGATCA |
| | CCGAAGTCAA | GCAGCATAGG | GCTCGGT | |

Figure S1: Sequences used in this research.

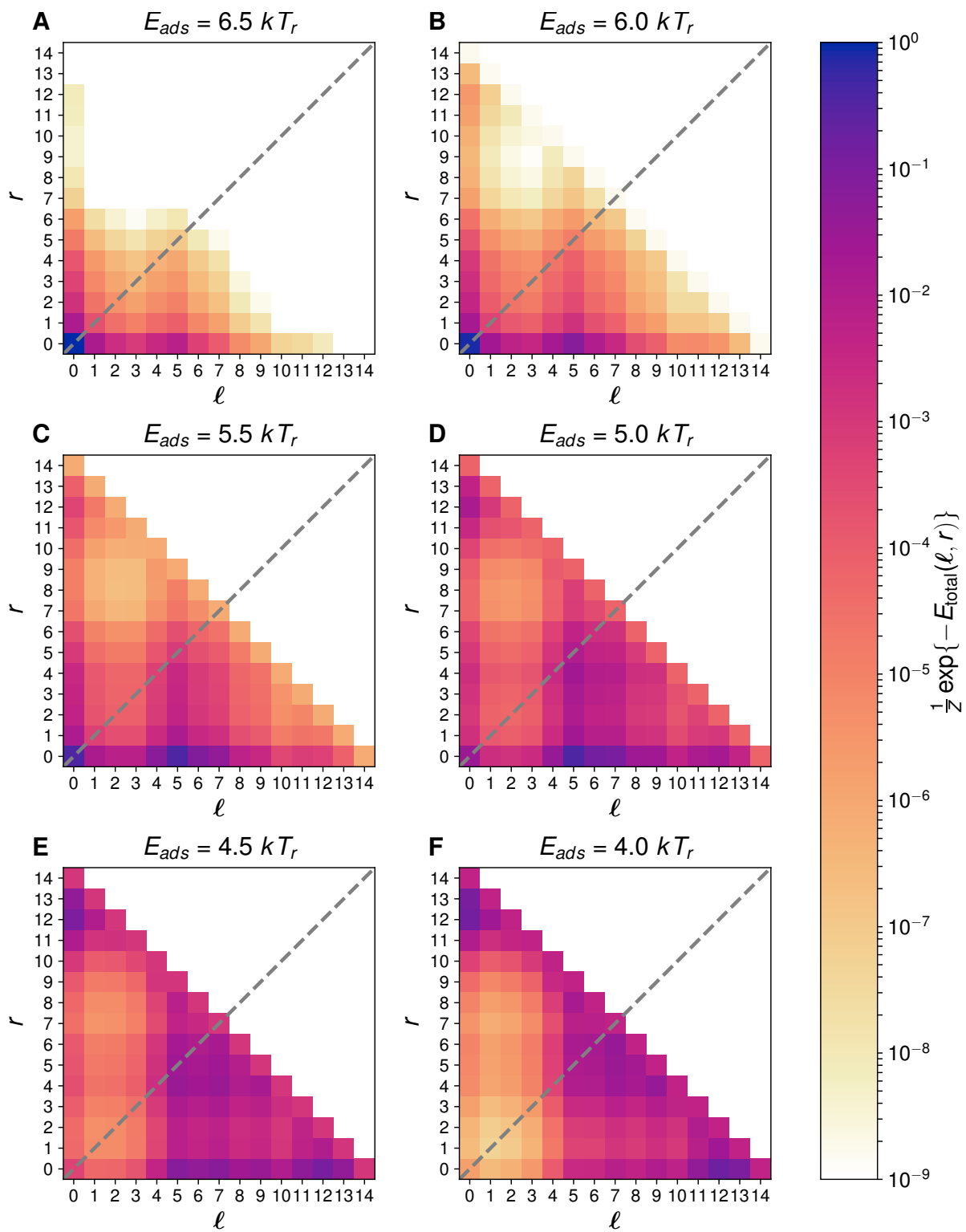


Figure S2: Relative occupancies of the 601 nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

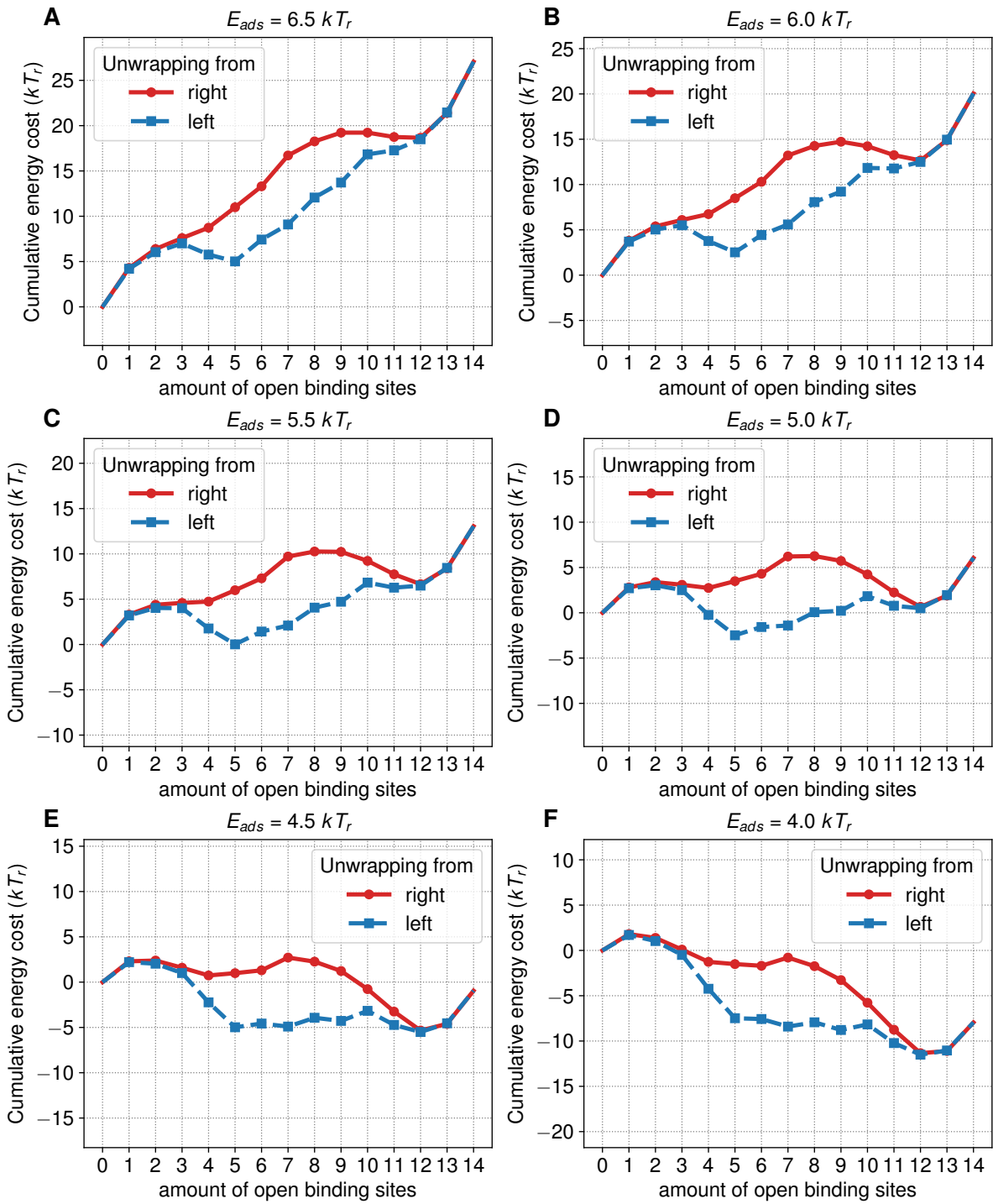


Figure S3: Cumulative energies for left (blue) and right (red) unwrapping of the 601 nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

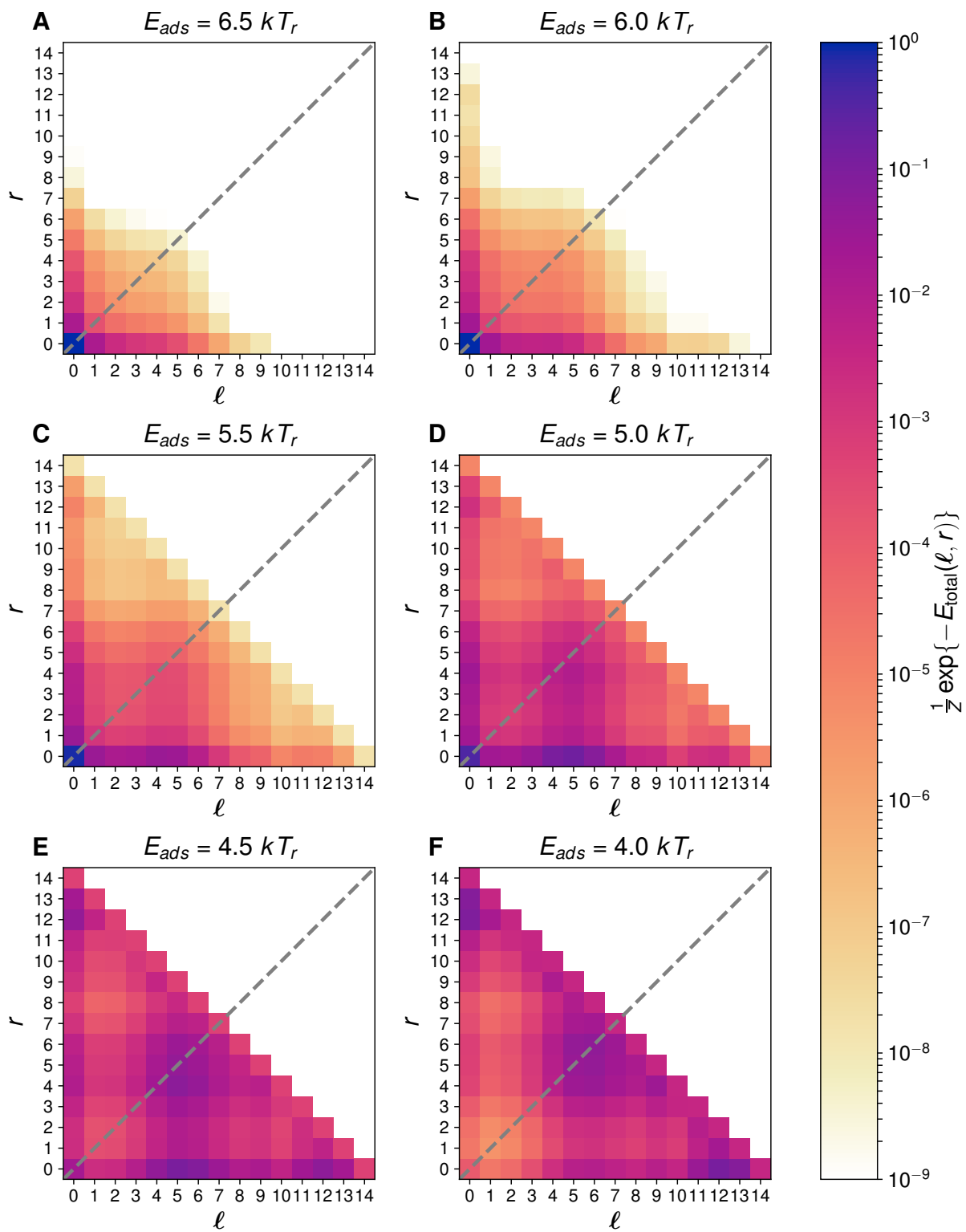


Figure S4: Relative occupancies of the 601RTA nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

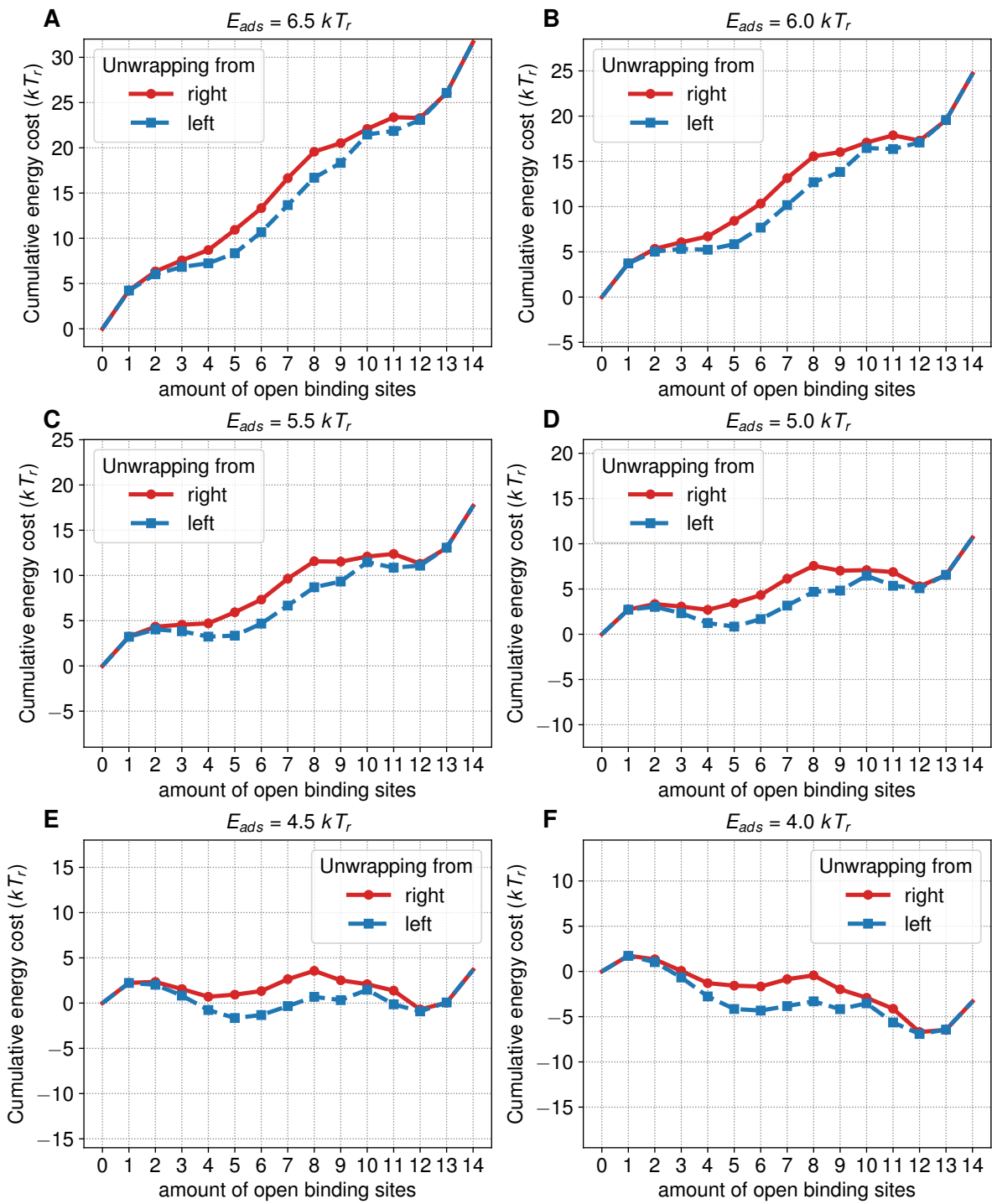


Figure S5: Cumulative energies for left (blue) and right (red) unwrapping of the 601RTA nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

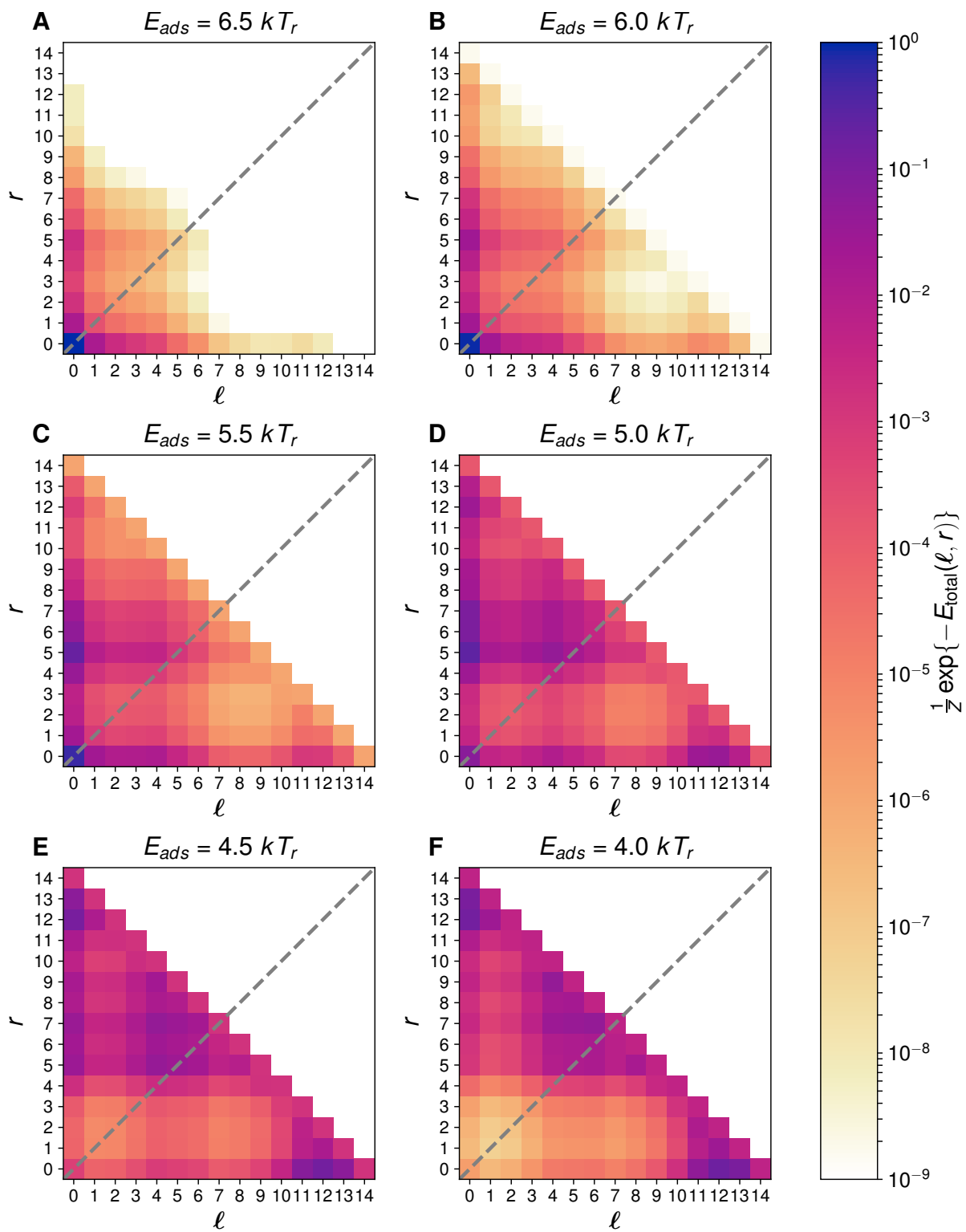


Figure S6: Relative occupancies of the 601MF nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

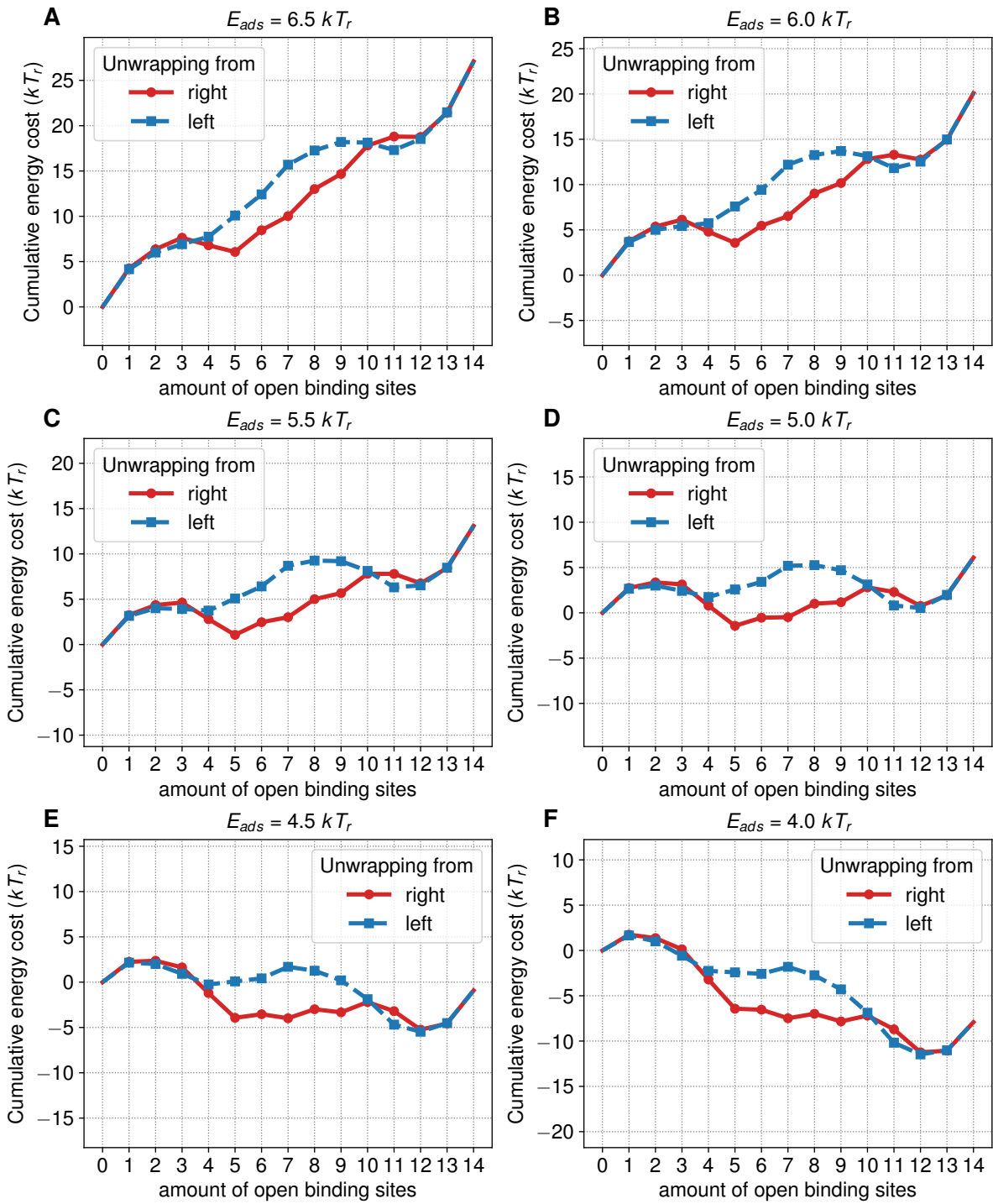


Figure S7: Cumulative energies for left (blue) and right (red) unwrapping of the 601MF nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

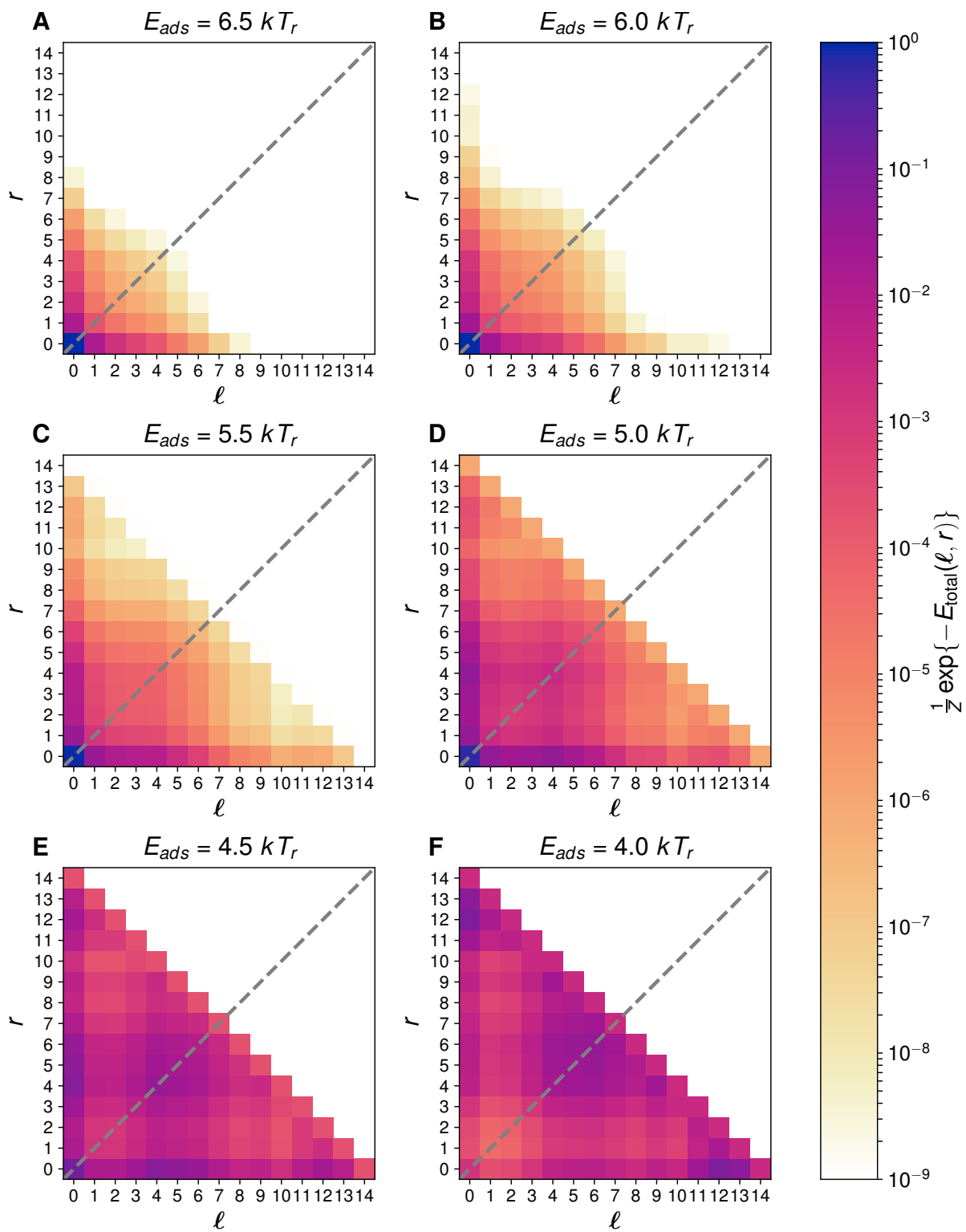


Figure S8: Relative occupancies of the 601L nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

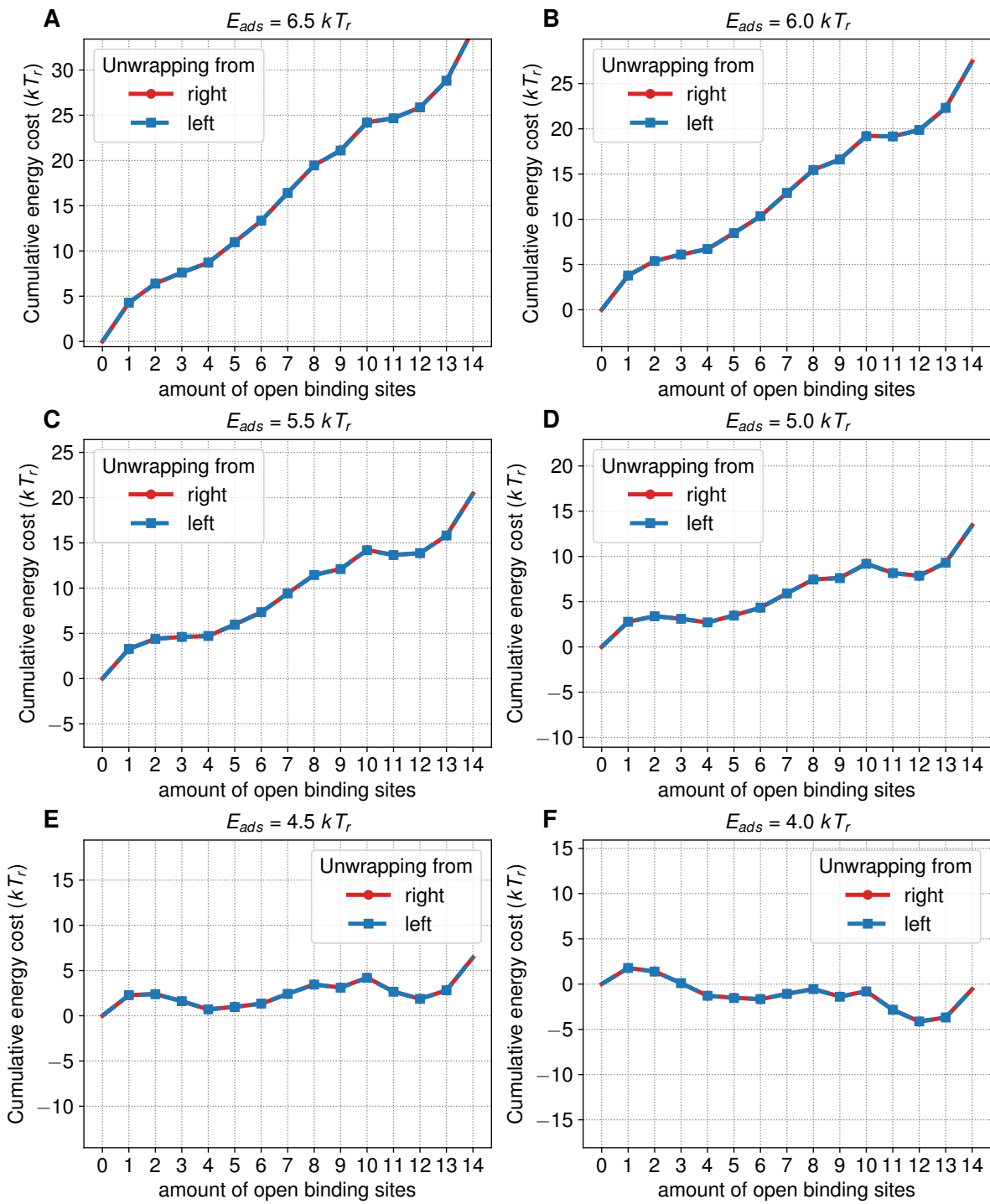


Figure S9: Cumulative energies for left (blue) and right (red) unwrapping of the 601L nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

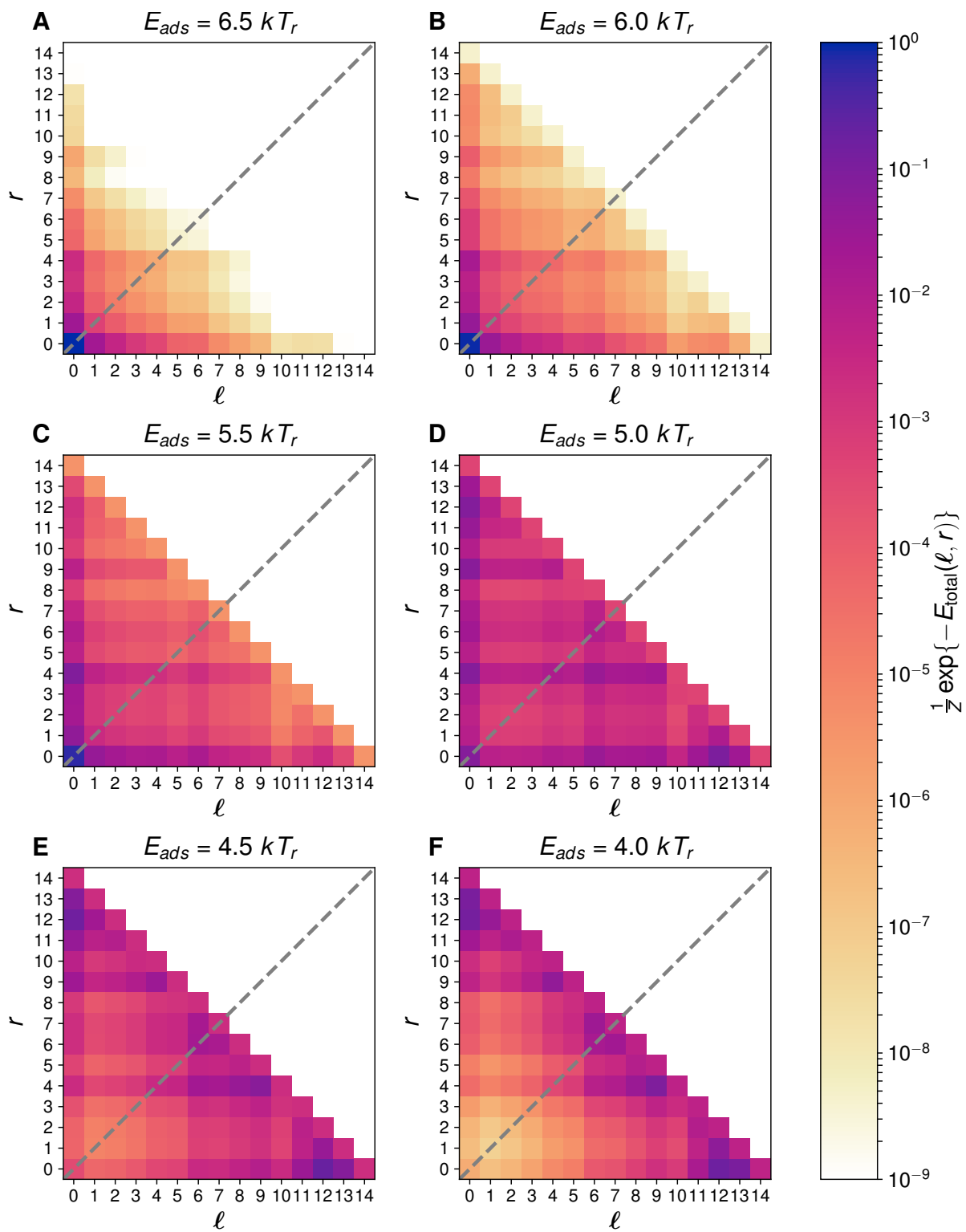


Figure S10: Relative occupancies of the 5S nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

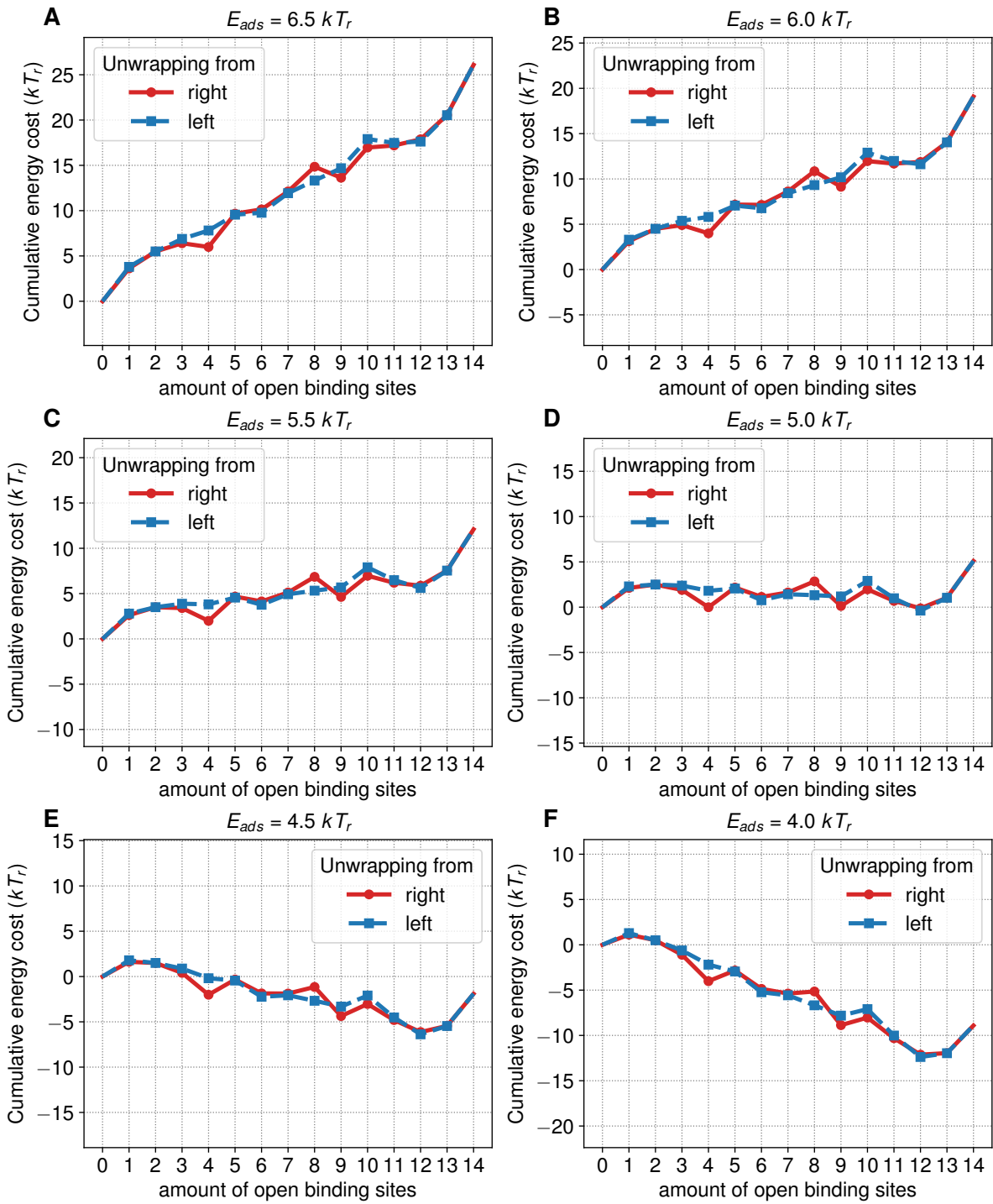


Figure S11: Cumulative energies for left (blue) and right (red) unwrapping of the 5S nucleosome for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

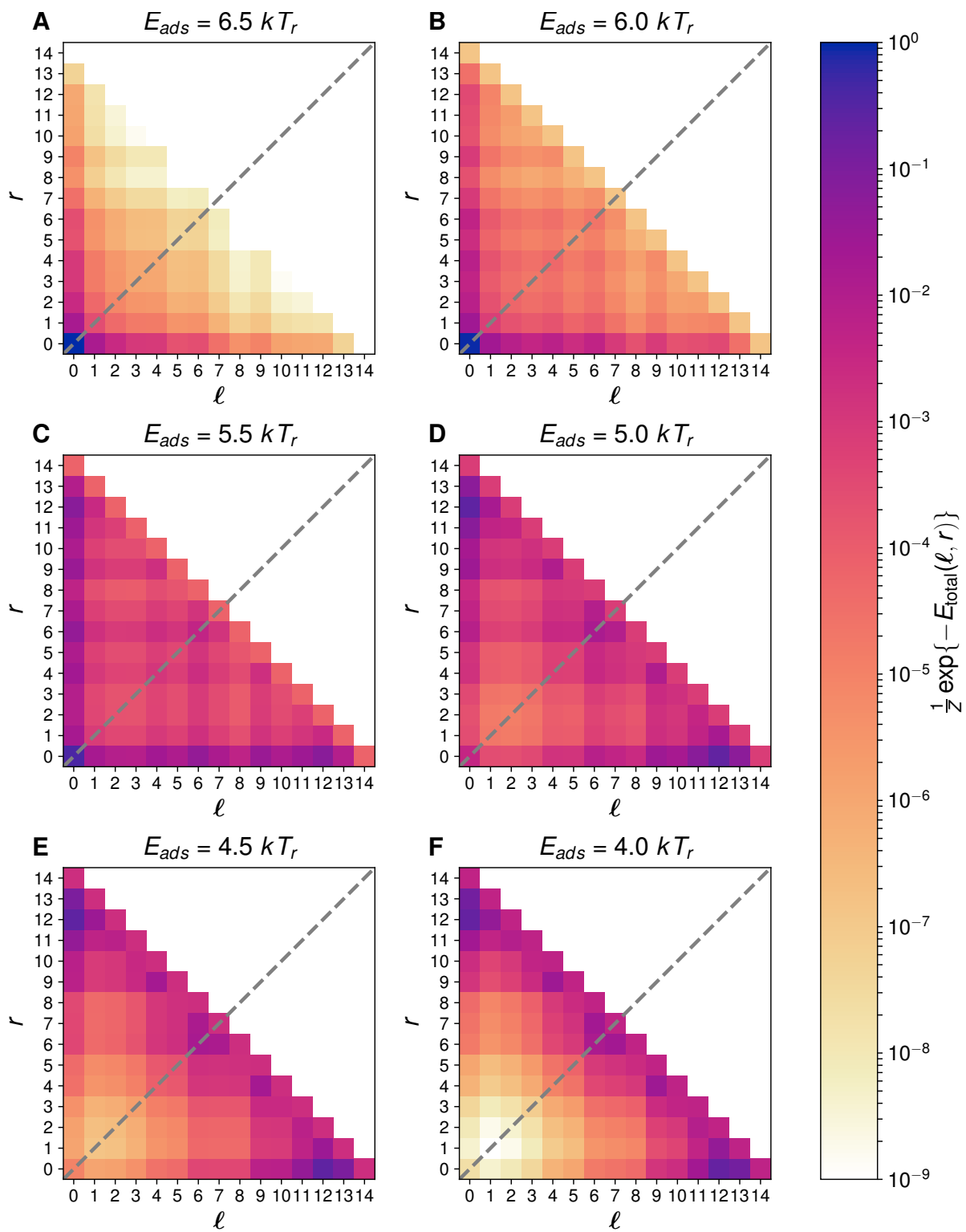


Figure S12: Relative occupancies of the nucleosome wrapped with (theoretical) uniform DNA for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

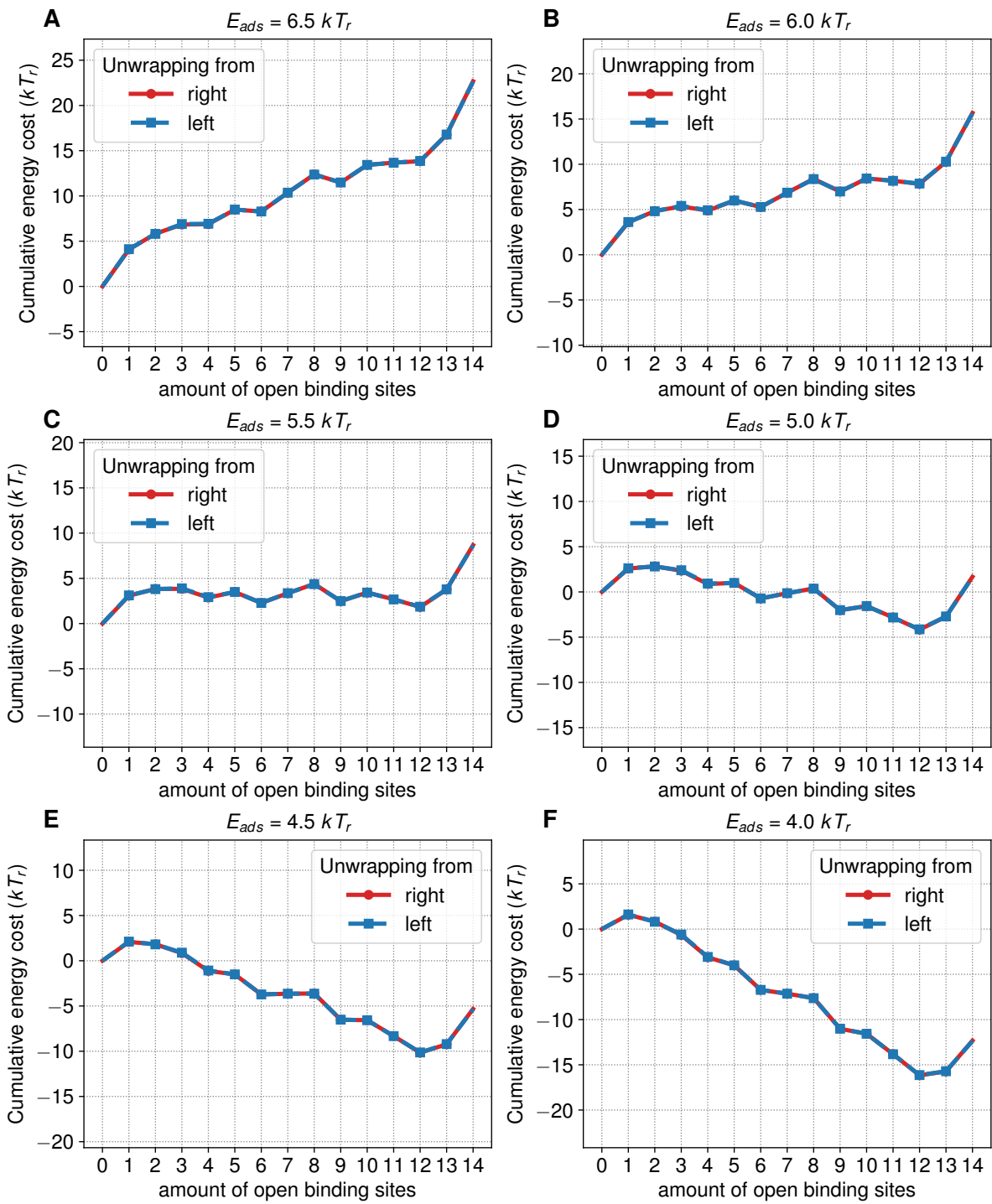


Figure S13: Cumulative energies for left (blue) and right (red) unwrapping of the nucleosome wrapped with (theoretical) uniform DNA for adsorption energies ranging from $6.5 kT_r$ to $4.0 kT_r$.

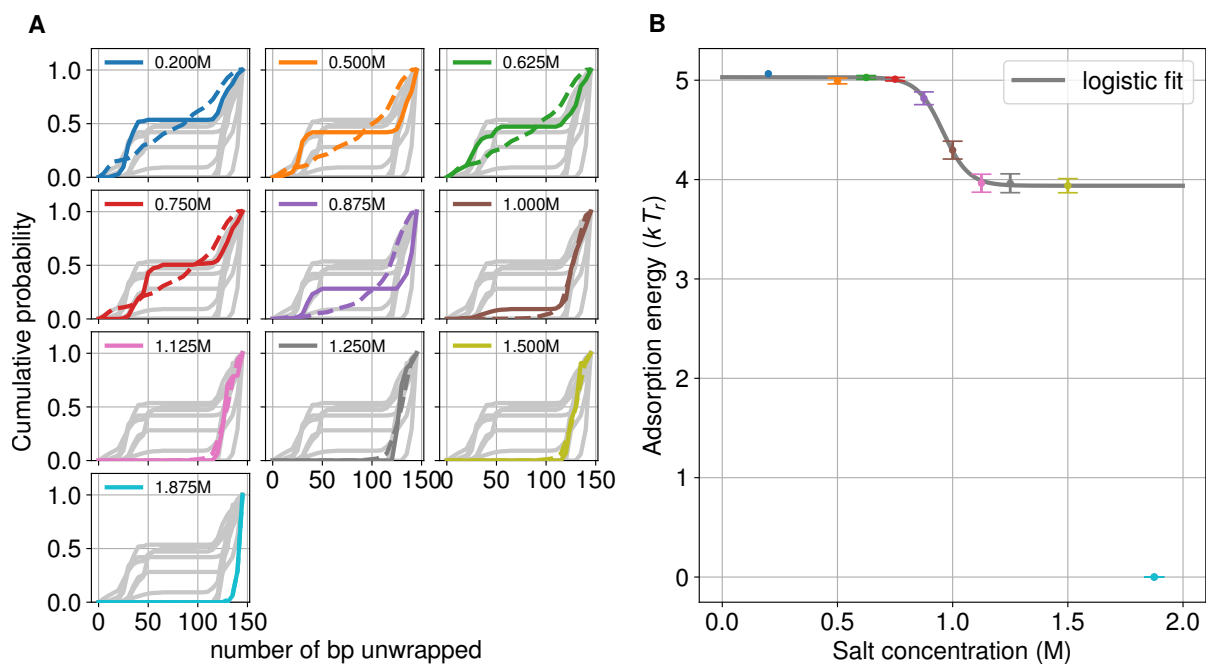


Figure S14: (A) The experimental cumulative probabilities (solid lines) for different salt concentrations, and the best fitting probabilities from our model (dashed lines) for the 5S nucleosome. (B) The adsorption energy in our model from the fits in (A) as a function of the experimental salt concentrations (colored circles) and the best fitting logistic curve. For this fitting the point at 1.875 M was not taken into account. The error bars are the standard errors of the fitting on the left.

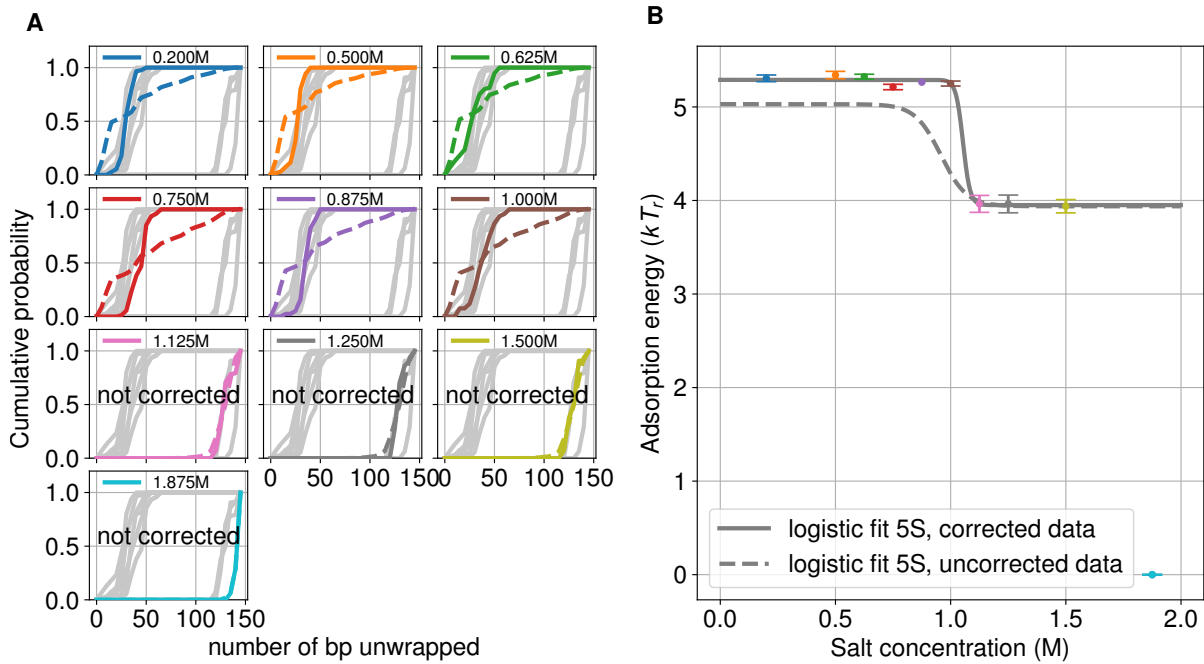


Figure S15: (A) The corrected (by rescaling the original data so that the largest plateau has a value of one, up to salt concentrations of 1.0 M) experimental cumulative probabilities of the 5S nucleosome (solid lines) for different salt concentrations, and the best fitting probabilities from our model (dashed lines). (B) The adsorption energy in our model from the fits in (A) as a function of the experimental salt concentrations (colored circles) and the best fitting logistic curve to the corrected data (solid curve) and the fit of the uncorrected data from Figure S14 (dashed curve). For this fitting the point at 1.875 M was not taken into account. The error bars are the standard errors of the fitting on the left.

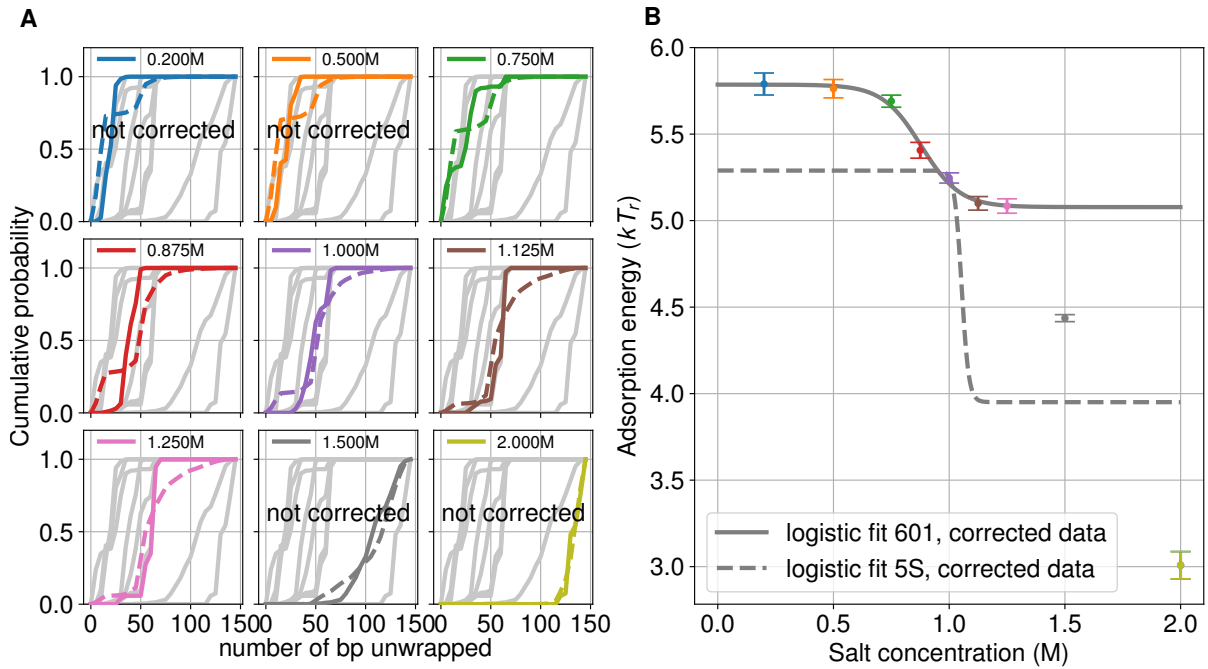


Figure S16: (A) The corrected (by rescaling the original data so that the largest plateau has a value of one, up to salt concentrations of 1.25 M) experimental cumulative probabilities of the 601 nucleosome (solid lines) for different salt concentrations, and the best fitting probabilities from our model (dashed lines). (B) The adsorption energy in our model from the fits in (A) as a function of the experimental salt concentrations (colored circles) and the best fitting logistic curve to the corrected 601 data (solid curve) and the best fitting logistic curve to the corrected 5S data from Figure S15 (dashed curve). For this fitting the points at 1.5 M and up were not taken into account. The error bars are the standard errors of the fitting on the left.