

Supplementary Information for Two-photon-absorption DNA sensitization via solvated electrons production: Unraveling the photochemical pathways by molecular modeling and simulation

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Figure S1) Jablonski Diagram for the photoionization processes extracted from 20 MD snapshots for the four stable interaction modes. A) Intercalation b) Alternative intercalation c) Minor groove binding d) Alternative minor groove binding. The square represents the energy of the solvated electrons in the limiting 3.3 and 3.6 eV

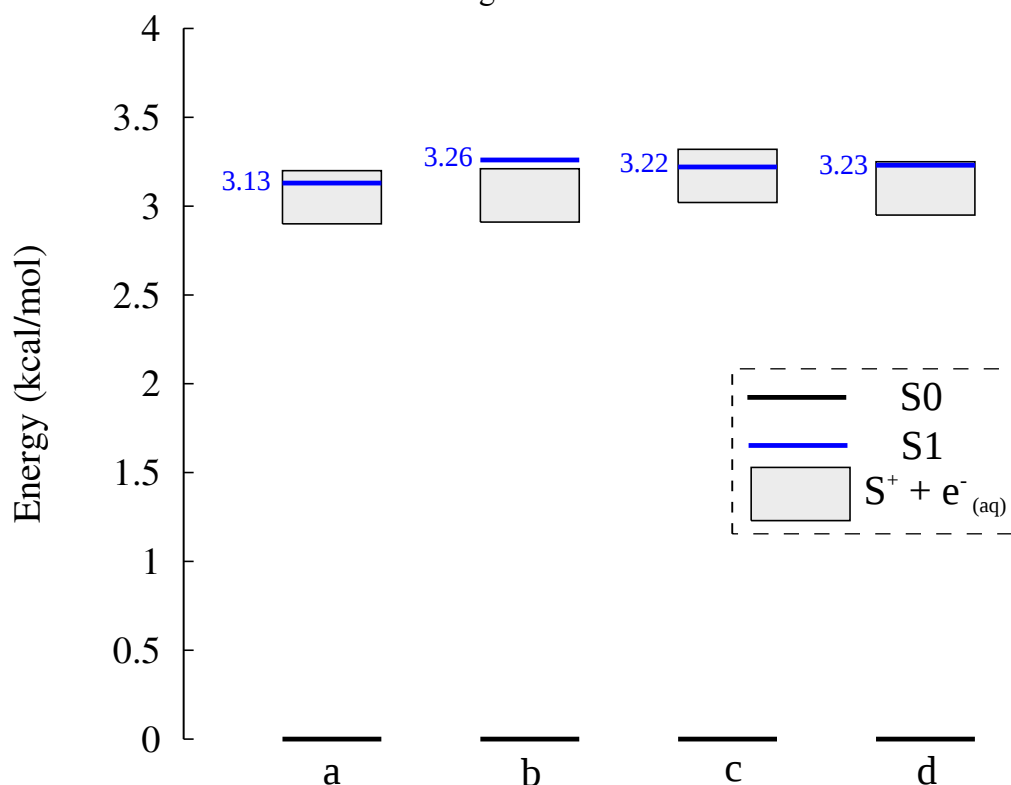


Figure S2) DNA minor groove width and depth for the four stable interaction mode as obtained using Curves+ code

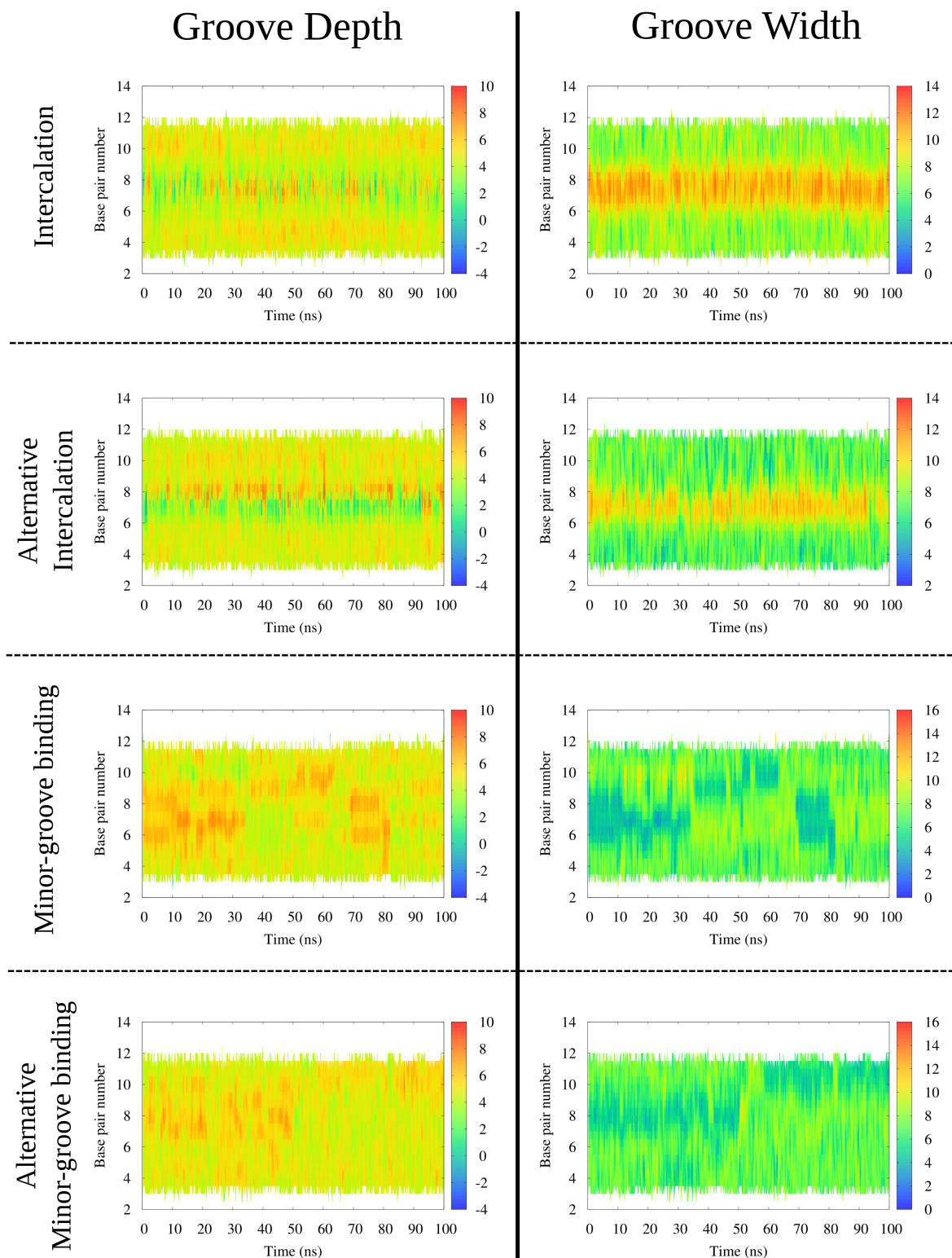


Figure S4) B-DNA hemix bending for the four interaction modes obtained with the Curves+ code

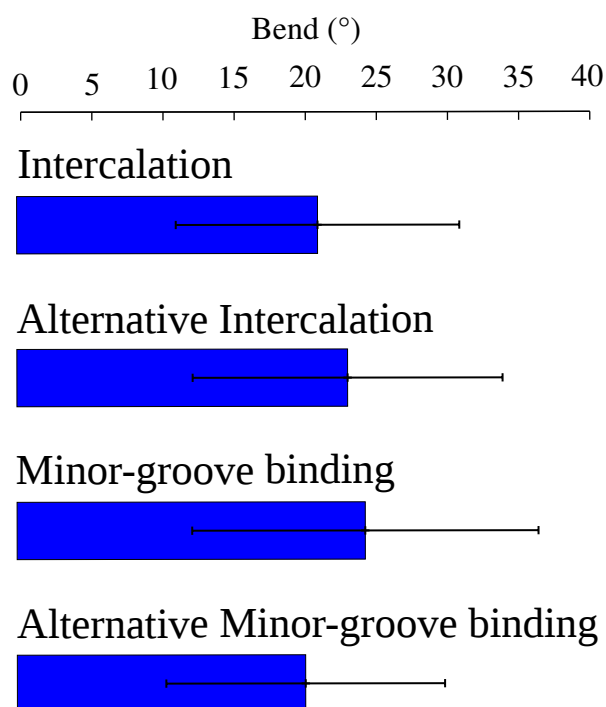
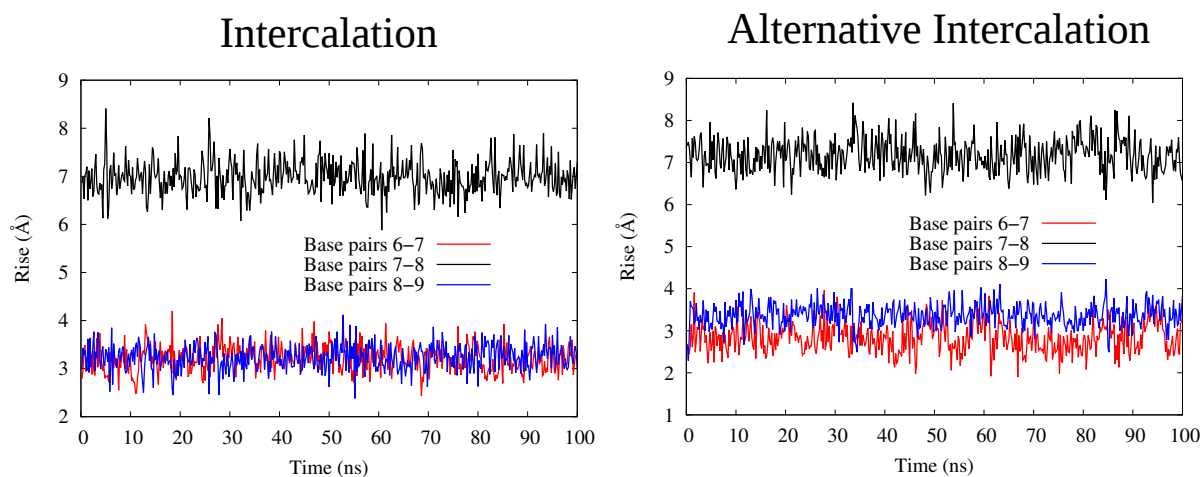


Figure S5) Time series of the base-pair rise for the intercalation and alternative intercalation obtained with the Curves+ code BMEMC is between base pair 7 and 8



References

1) R. Lavery, M. Moakher, J.H. Maddocks, D. Petkeviciute, K. Zakrzewska
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