

SUPPLEMENTARY MATERIAL

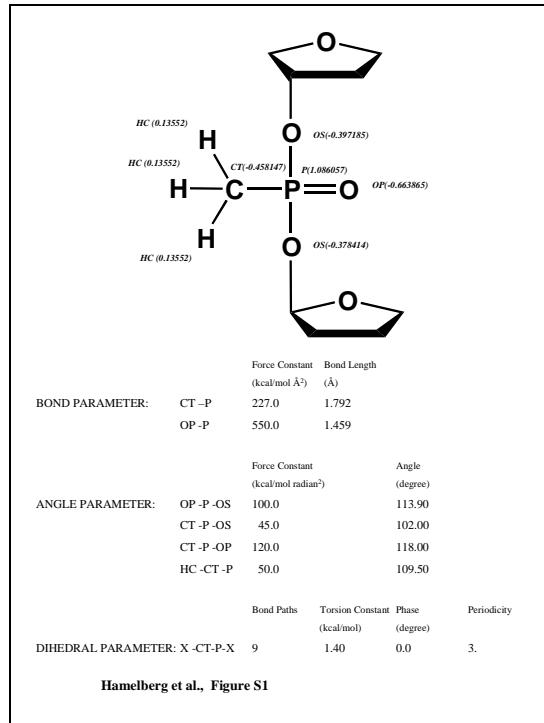


Figure S1. The atom types and partial atomic charges of the methylphosphonate moiety were determined as described in the Method section (top). The additional force field parameters used (below).

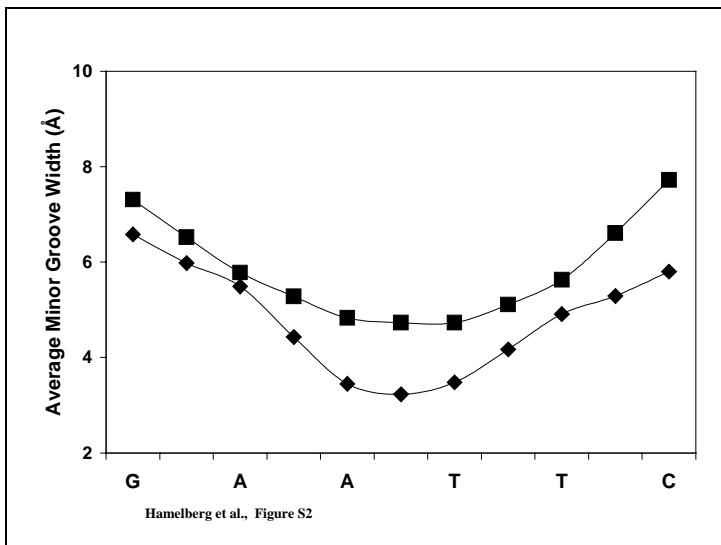


Figure S2. Effect of phosphate neutralization on the time-average minor groove width profile of the central A-tract of the AATT duplexes. The black squares show the unmodified AATT duplex, and the black diamonds show the alternating methylphosphonate modified duplex.

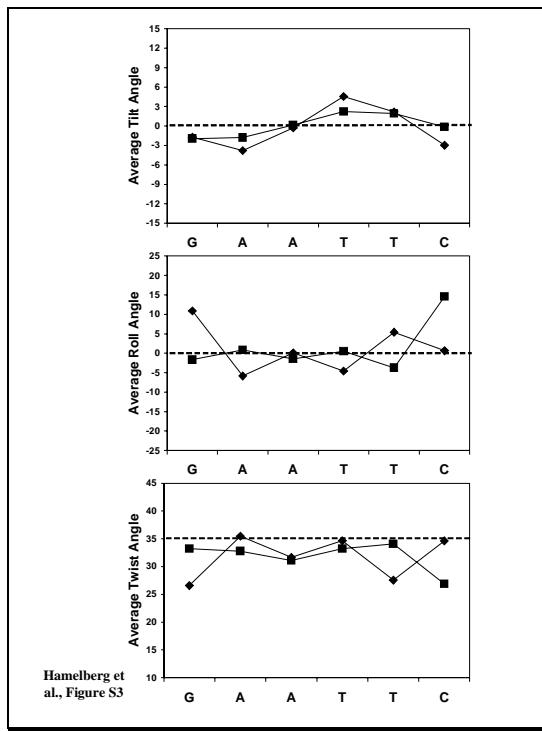


Figure S3. Plots of tilt, twist and roll angles of AATT duplexes. Unmodified AATT duplex (squares) and M_AATT_ALT (diamonds).