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Computational simulations of PDMAEMA for the transport of nucleic acids

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Abstract: It has been previously reported the use of poly(dimethylaminoethyl methacrylate) (PDMAEMA) polymer brushes for the design of gene delivery vectors due to high loading levels of small plasmids. Unanswered questions concerning the PDMAEMA-RNA/DNA interactions such as the increased stability of PDMAEMA-RNA complexes relative to polymer complexes with DNA can be investigated through molecular simulations. In this work the parameter set GROMOS 54a7 was used to perform atomistic molecular dynamics simulations of the PDMAEMA polymer brush in close contact with molecules of ribonucleotides, in order to investigate the possible influence of the genetic sequence on the adhesion of nucleic acids to the polymer. During the simulated time all ribonucleotides tested (deoxyadenylate, deoxycytidylate, deoxyguanylate and uridylate) adhere strongly to the polymer surface, showing no qualitative differences in their interactions.