Conformational behavior of a semiflexible dipolar chain with a variable relative size of charged groups via molecular dynamics simulations.

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Supporting information.

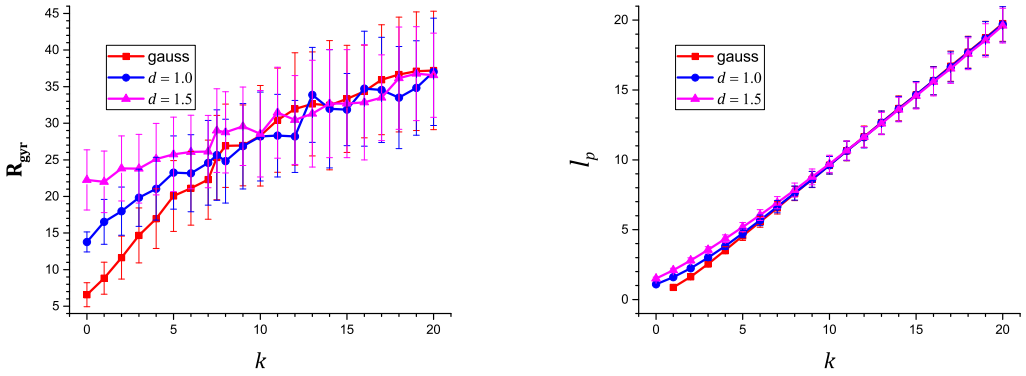

Figure S1. Radius of gyration R_{gyr} (left) and persistence length l_p (right) as functions of rigidity k in the case of the ideal chain (gauss) and for uncharged chains in good solvent with different dipole length $d = 1.0$ and 1.5.

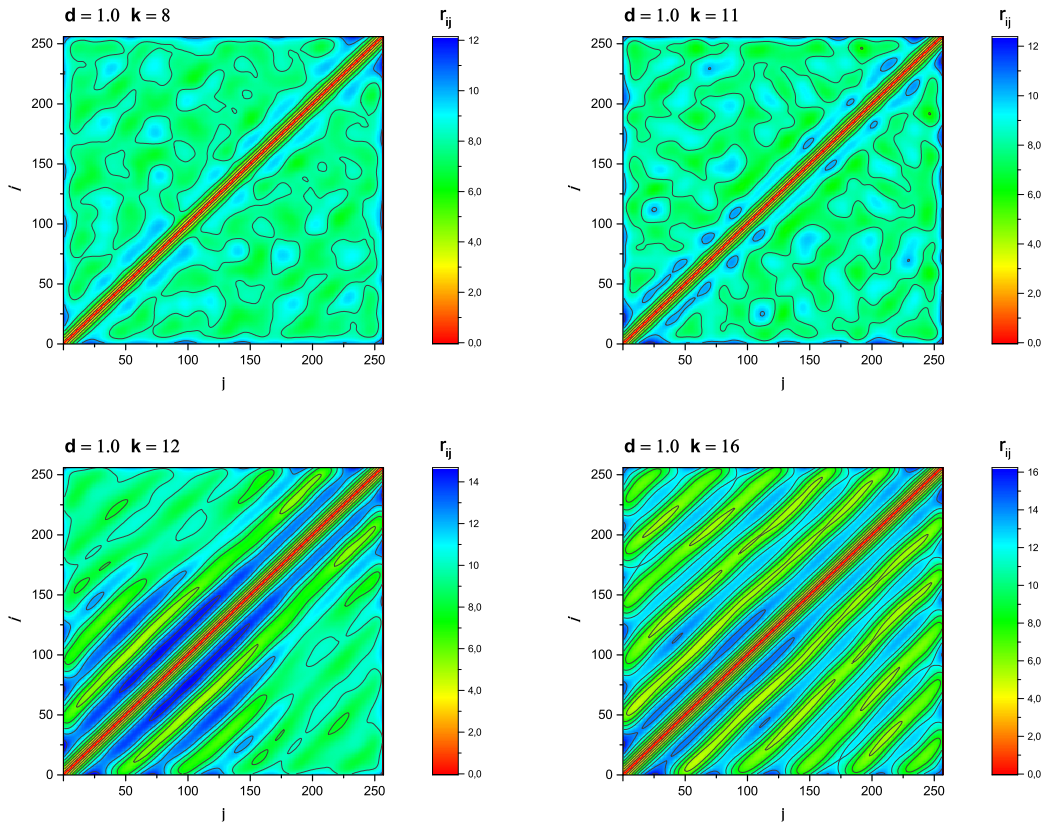

Figure S2. Distance map for backbone units with dipole length $d = 1$ for different $k = 8, 11, 12, 16$ at $\lambda = 10$.

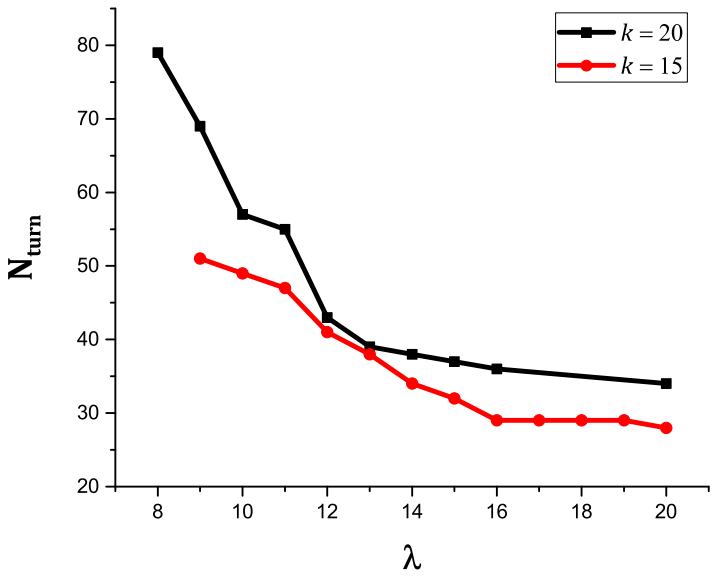

Figure S3. Number of turns of the torus as function of λ at different k and $d = 1$

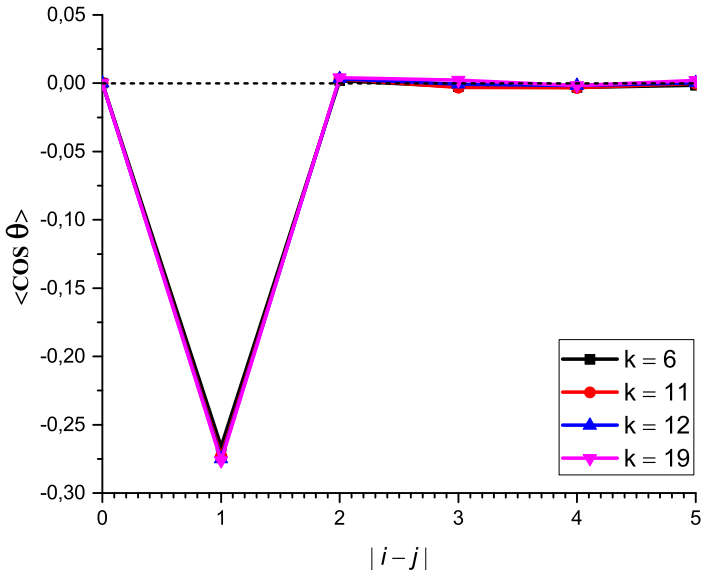

Figure S4. The average cosine between dipoles as function of number along chain for different k at $\lambda = 10$ and $d = 1$.

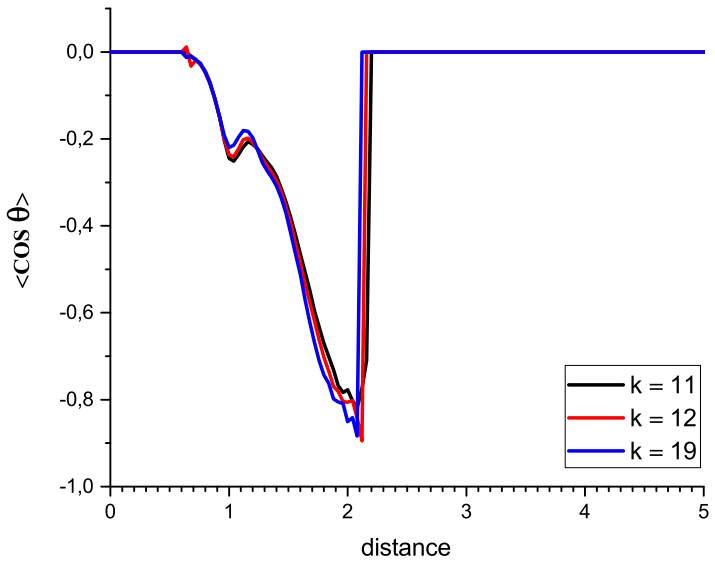

Figure S5. The average cosine between dipoles neighboring along the chain along as function of distance in space for different k at $\lambda = 10$ and $d = 1$.

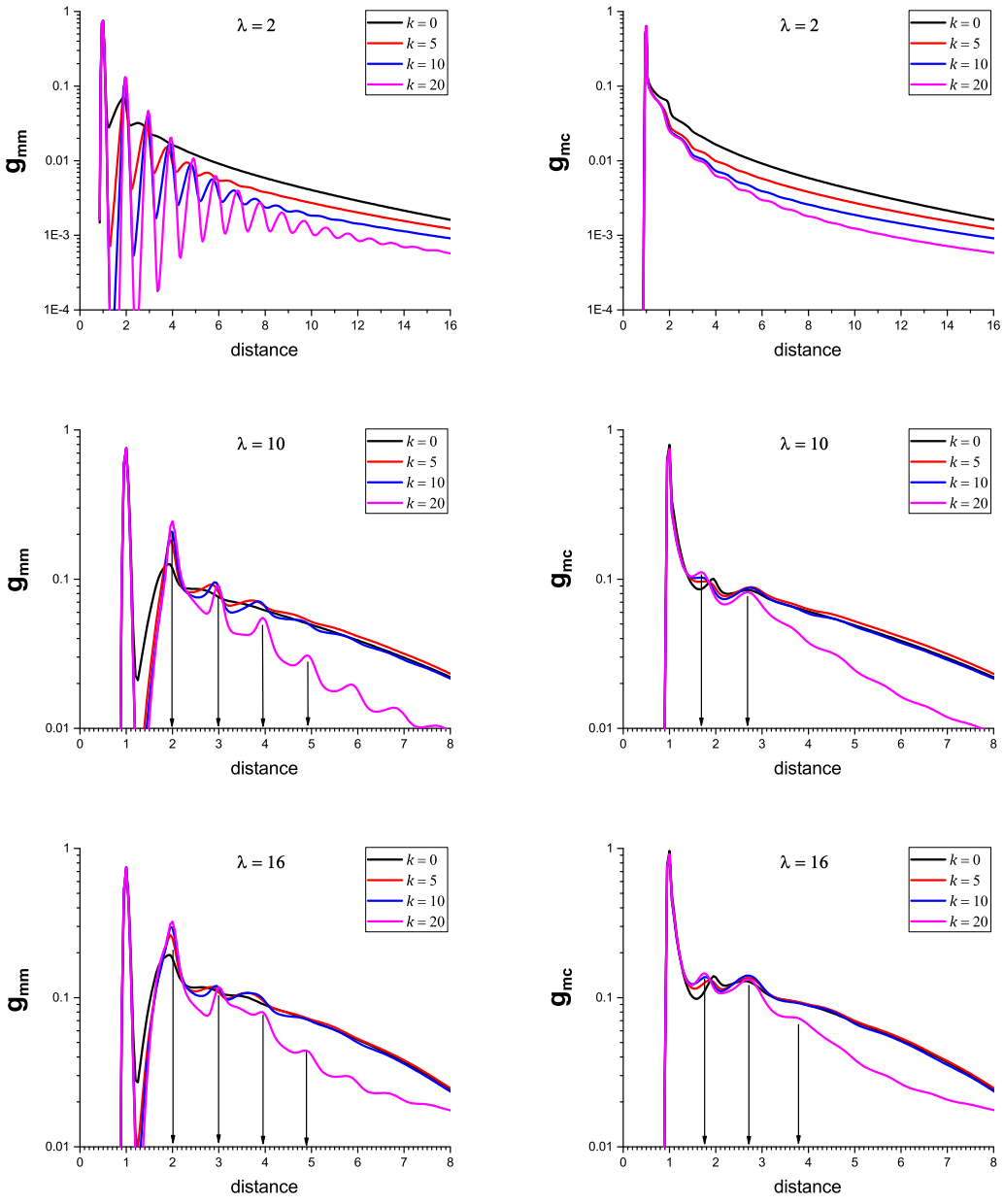

Figure S6. Radial distribution functions of backbone beads relative to each other, g_{mm}, as well as relative to side beads, g_{mc}, for different λ and k at $d = 1$

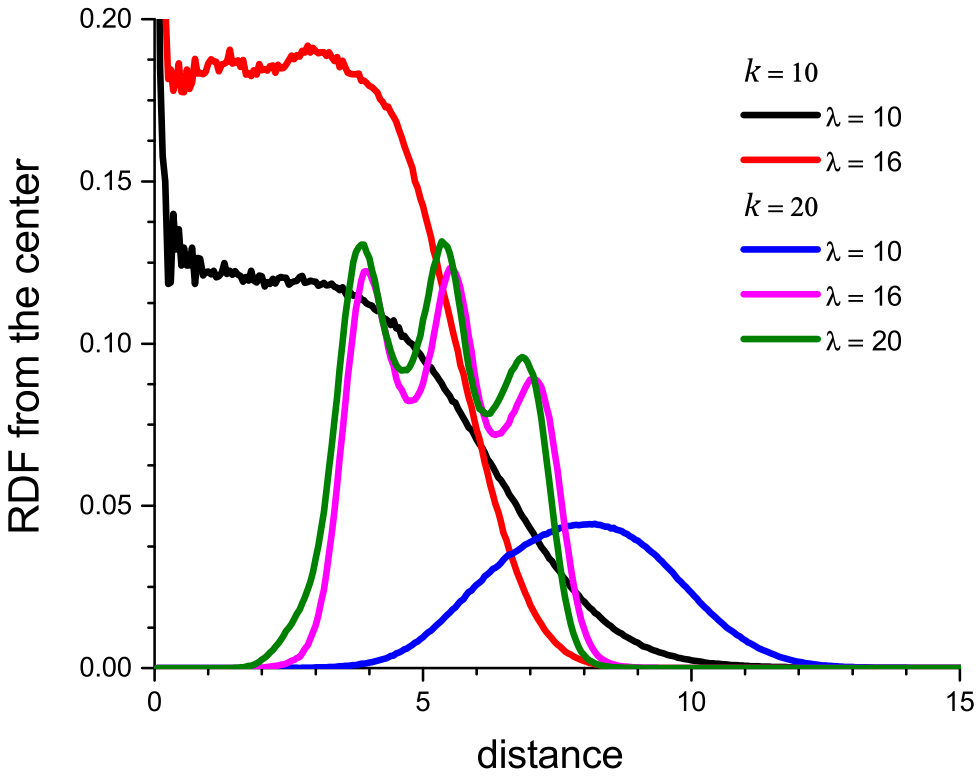

Figure S7. Radial distribution functions of backbone beads relative to the center of mass of the chain for different λ and k at $d = 1$

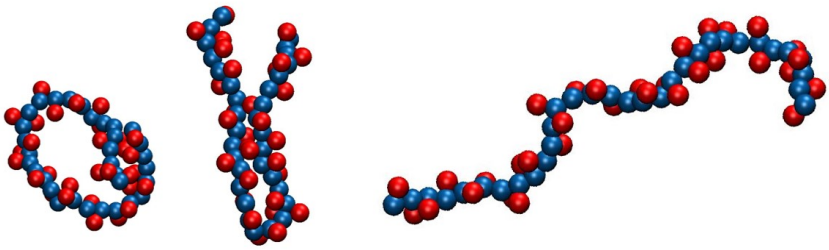

Figure S8. Snapshots of dipolar chain of rigidity $7 \leq k \leq 14$ at $\lambda = 10$, $N = 32$. There are metastable states such as circle, hairpin and extended chain.

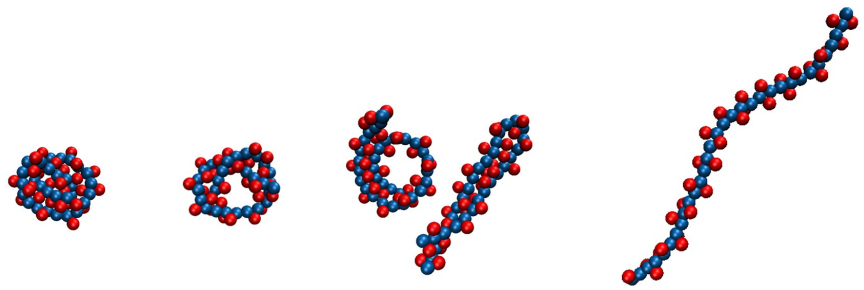

Figure S9. Snapshots of dipolar chain at $\lambda = 20$, $N = 32$. There are loose globule ($k = 15$), knots with trefoil knot ($k = 26$), hairpin with short-living torus ($k = 34$) and rod ($k = 40$).

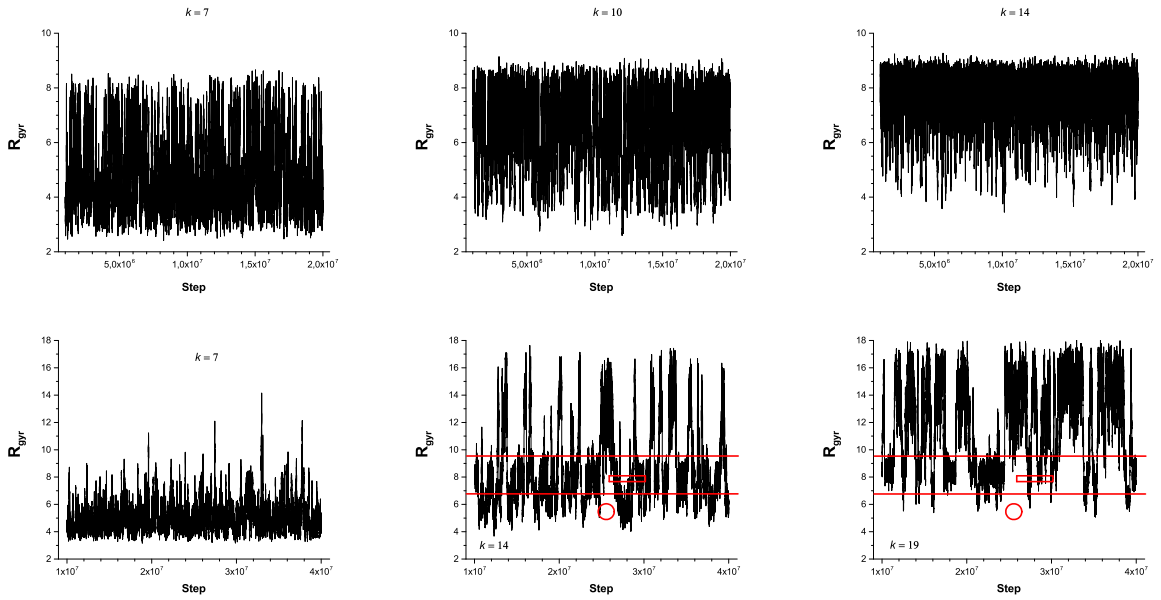

Figure S10. Dynamic exchange between toroidal structure, hairpin and extended chain in a typical run, as seen in the trace of radius of gyration as a function of time for different rigidity at $\lambda = 10$. Top: $N = 32$ and $k = 7, 10, 14$. Bottom: $N = 64$ and $k = 7, 14, 19$.

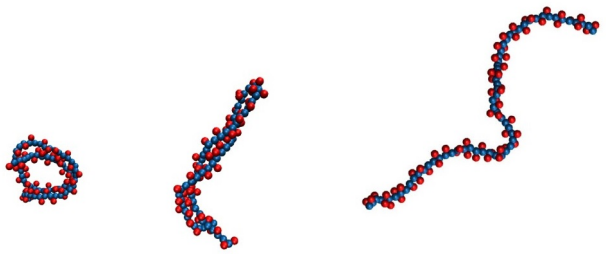

Figure S11. Snapshots of dipolar chain of rigidity $k = 7, 14, 19$ at $\lambda = 10$, $N = 64$.

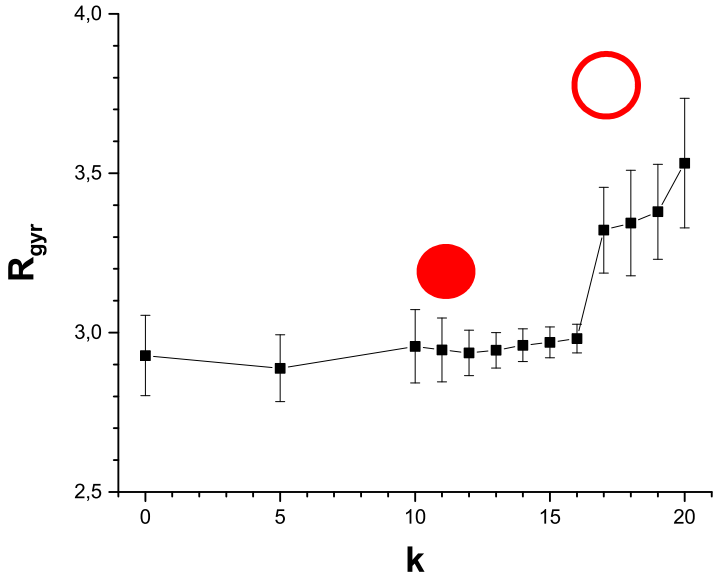

Figure S12. Radius of gyration R_{gyr} as function of rigidity k at $\lambda = 20$, $N = 64$.

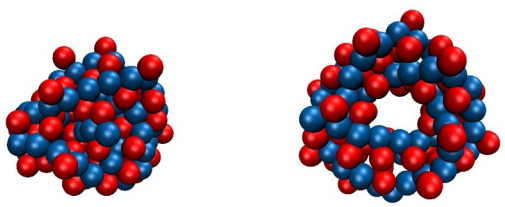

Figure S13. Snapshots of dipolar chain of rigidity $k = 14, 19$ at $\lambda = 20$, $N = 64$. There are globule and torus.

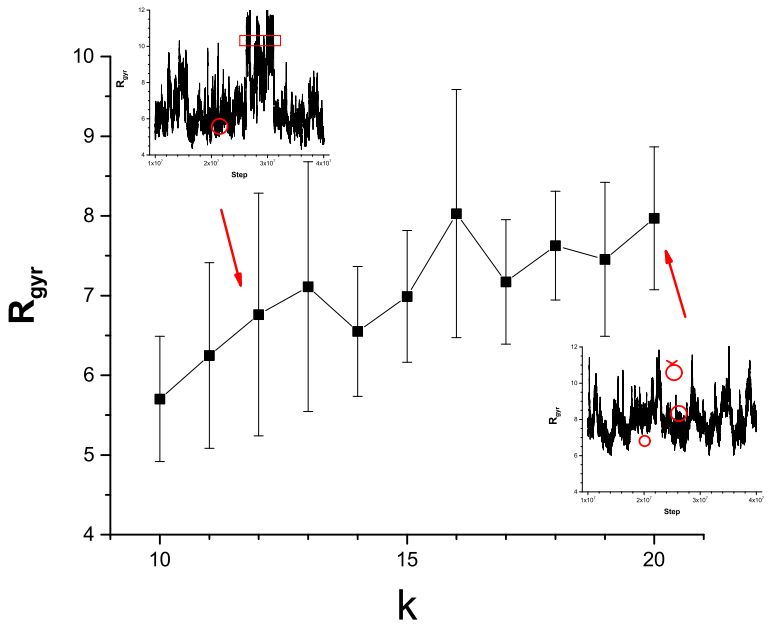

Figure S14. Radius of gyration R_{gyr} as function of rigidity k at $\lambda = 10$, $N = 128$.

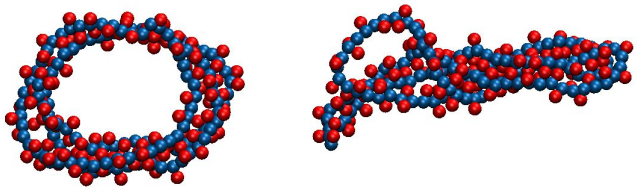

Figure S15. Snapshots of 128-chain for $11 \leq k \leq 20$, $\lambda = 10$, $d = 1$.

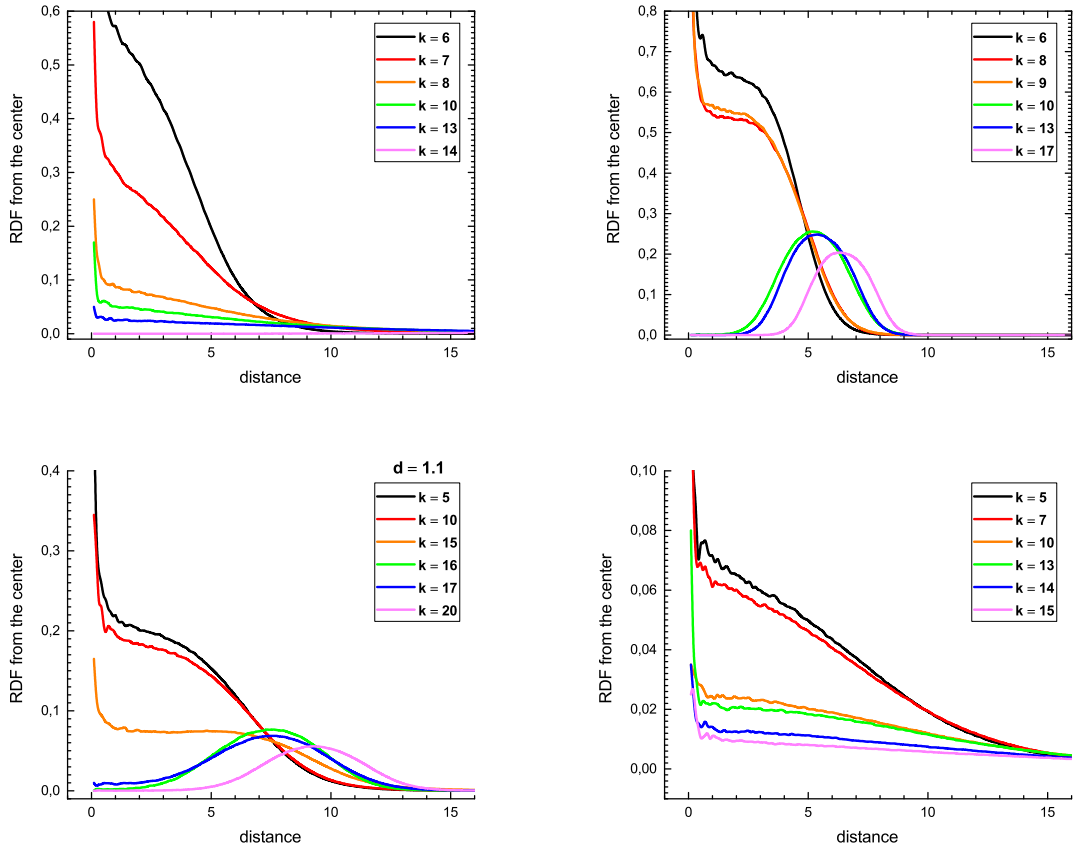

Figure S16. Radial distribution function (density) of backbone units from the center of mass of the chain for different k at $\lambda = 10$. From top to bottom: $d = 0.6, 0.7, 1.1, 1.2$.