Electronic Supplementary Material (ESI) for Soft Matter.

SUPPORTING INFORMATION

Crowded Solutions of Single-Chain Nanoparticles under Shear Flow

Maud Formanek[†,‡] and Angel J. Moreno[*,†,¶]

†*Centro de Física de Materiales (CSIC, UPV/EHU) and Materials Physics Center MPC, Paseo Manuel de Lardizabal 5, E-20018 San Sebastián, Spain*

‡*Sainsbury Laboratory, University of Cambridge, 47 Bateman Street, Cambridge CB2 1LR, United Kingdom*

¶*Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain*

E-mail: angeljose.moreno@ehu.es

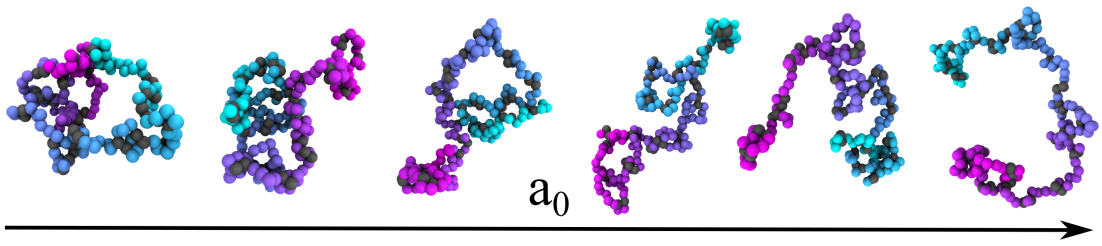

Figure S1. Typical snapshots of SCNPs in equilibrium and high dilution, with different values of the equilibrium asphericity a_0. From left to right, $a_0 = 0.17, 0.22, 0.34, 0.41, 0.47$ and 0.49. Grey beads are cross-linked monomers. The rest of the monomers are colored, from magenta to cyan, according to their position in the backbone of the linear precursor.

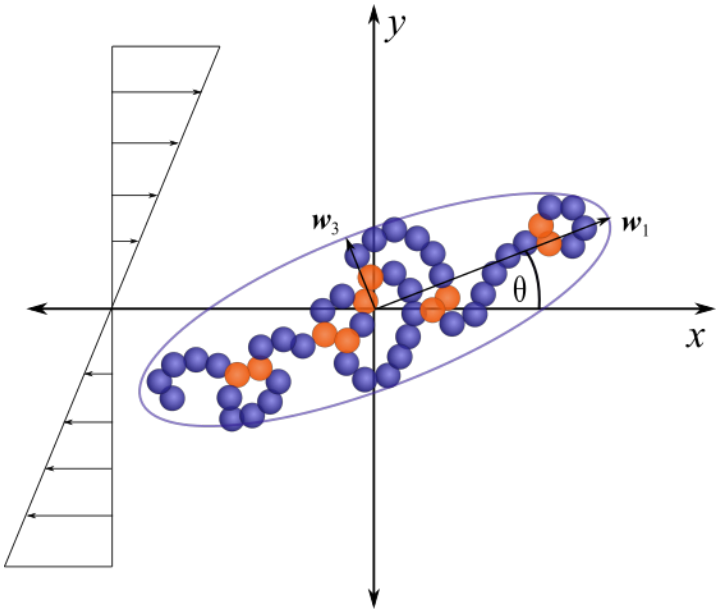

Figure S2. Scheme of the simulation setup, indicating the fluid velocity profile and the eigenvalues and eigenvectors of the gyration tensor. The x-axis is the flow direction, y is the gradient direction and z – perpendicular to the plane – is the vorticity direction. θ is the angle between the largest eigenvector of the gyration tensor, $\boldsymbol{w}_1$, and the direction of the flow. Reactive monomers forming cross-links are colored in orange, the rest are depicted in blue.

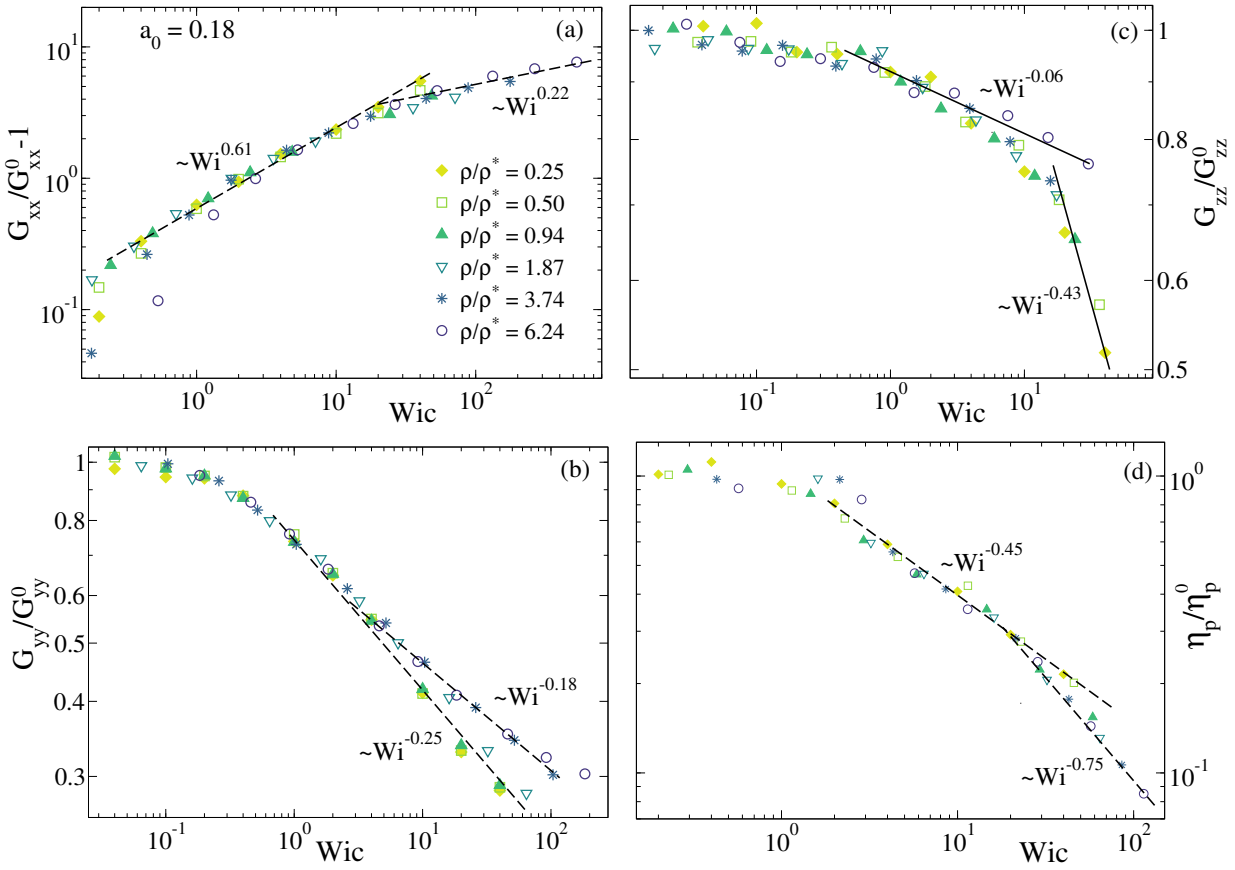

Figure S3. For the monodisperse solutions of SCNPs with low equilibrium asphericity $a_0 = 0.18$, diagonal components of the inertia tensor (a-c) and polymer contribution to the viscosity (d). Data sets are normalized by their values ($G^0_{\alpha\alpha}$, η^0_p) at the lowest simulated shear rate of their corresponding concentration (in all cases $\dot{\gamma} = 5 \times 10^{-5}$). Dashed lines represent power laws.

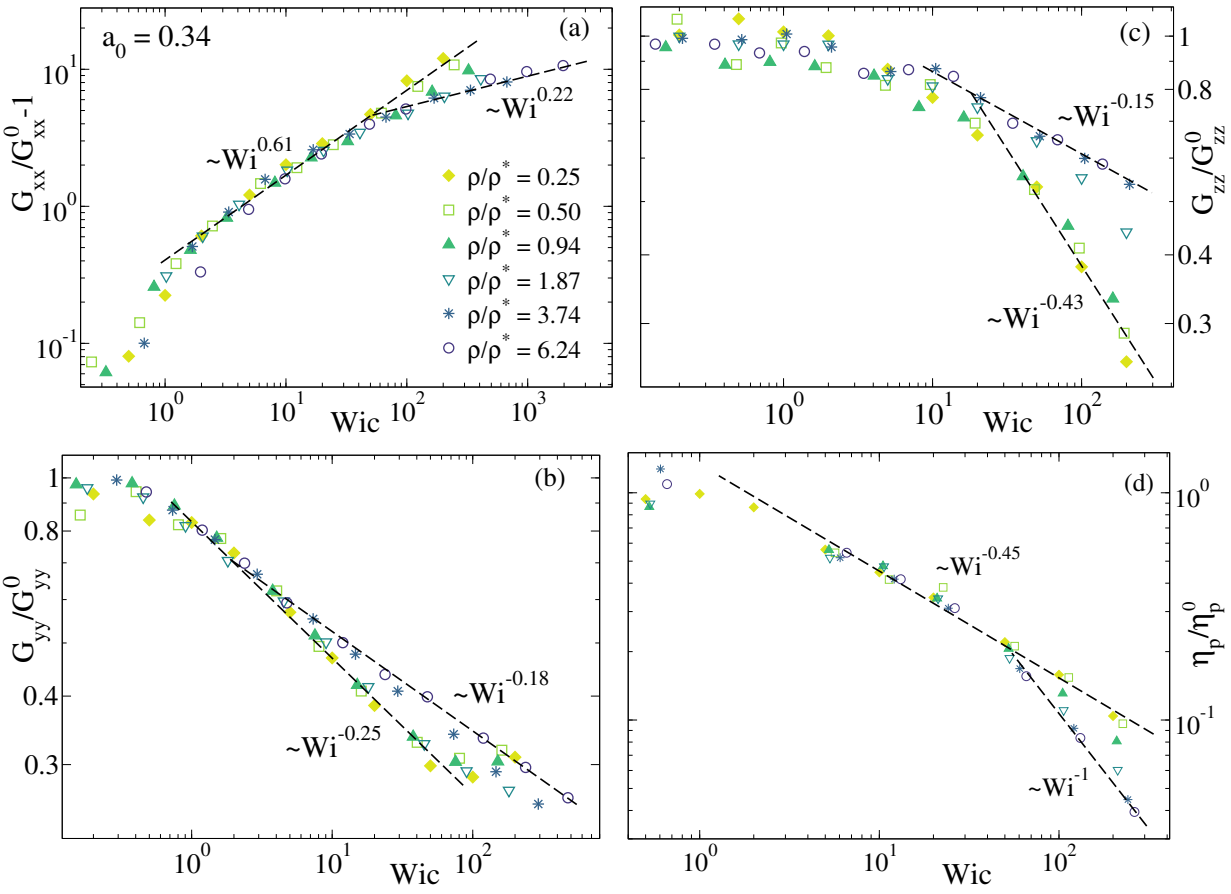

Figure S4. As Figure S3 for the SCNPs with middle equilibrium asphericity $a_0 = 0.34$.

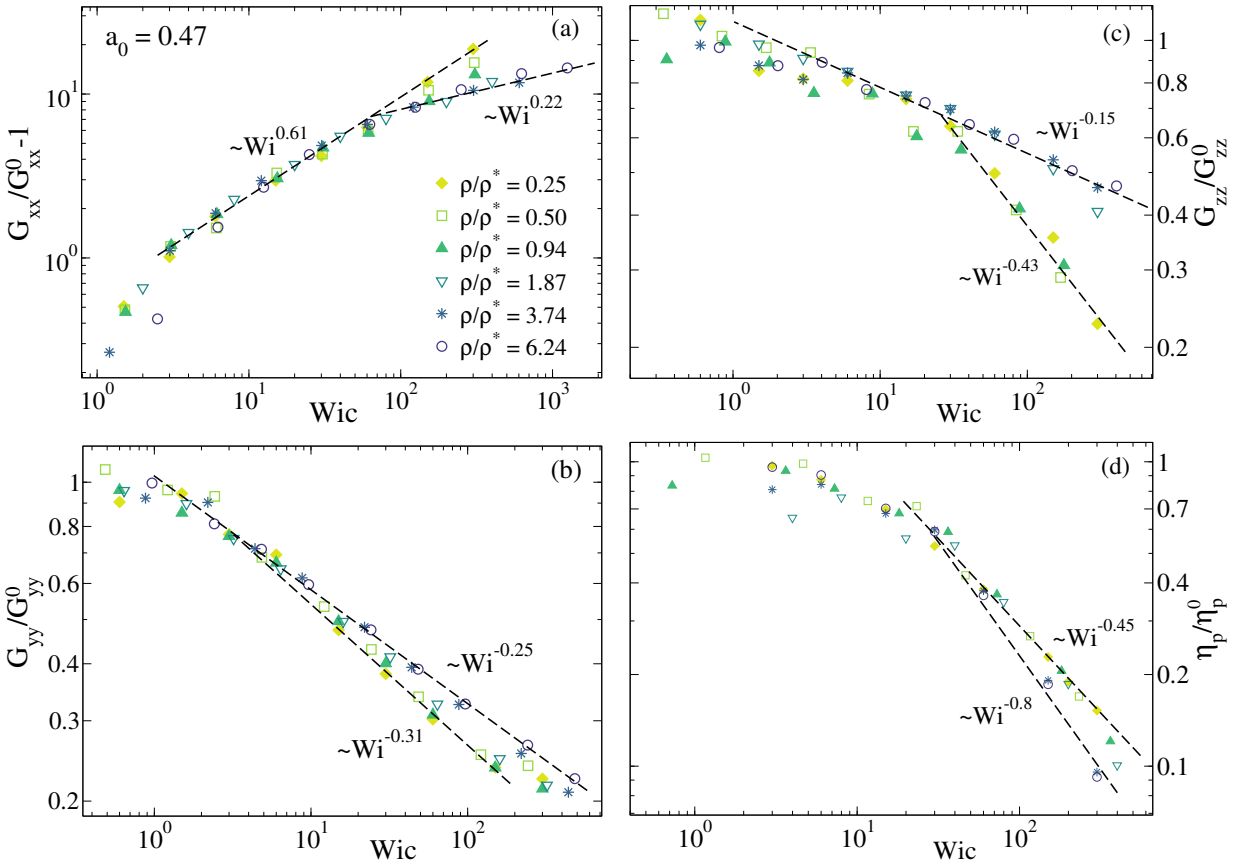

Figure S5. As Figure S3 for the SCNPs with high equilibrium asphericity $a_0 = 0.47$.

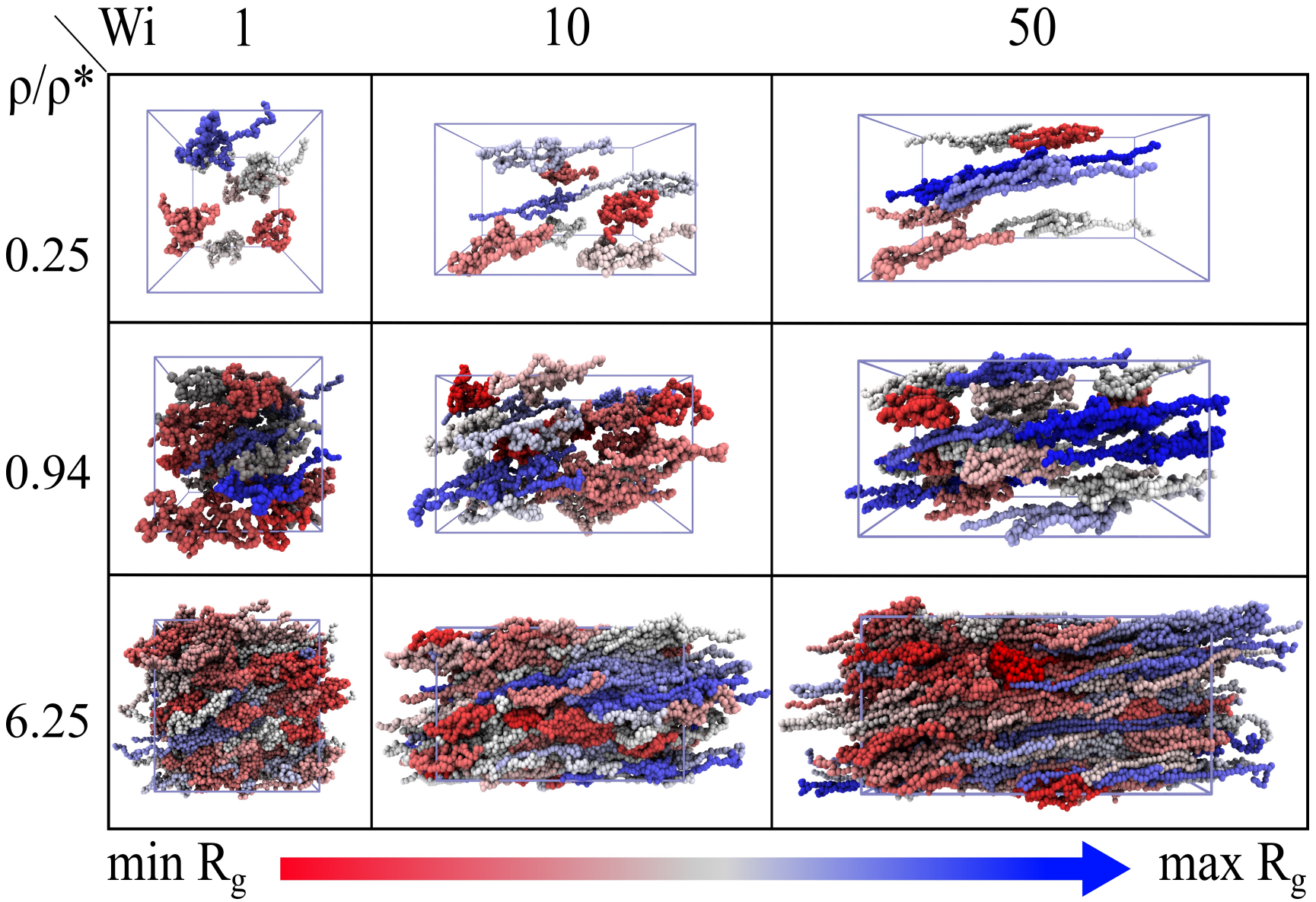

Figure S6. Snapshots of the simulation box for the monodisperse solution of SCNPs with low equilibrium asphericity $a_0 = 0.18$, at different values of the Weissenberg number and the concentration. All the SCNPs in the box are represented and they are colored according to their instantaneous radius of gyration (dark red to dark blue from lower to higher R_g, grey for medium size).

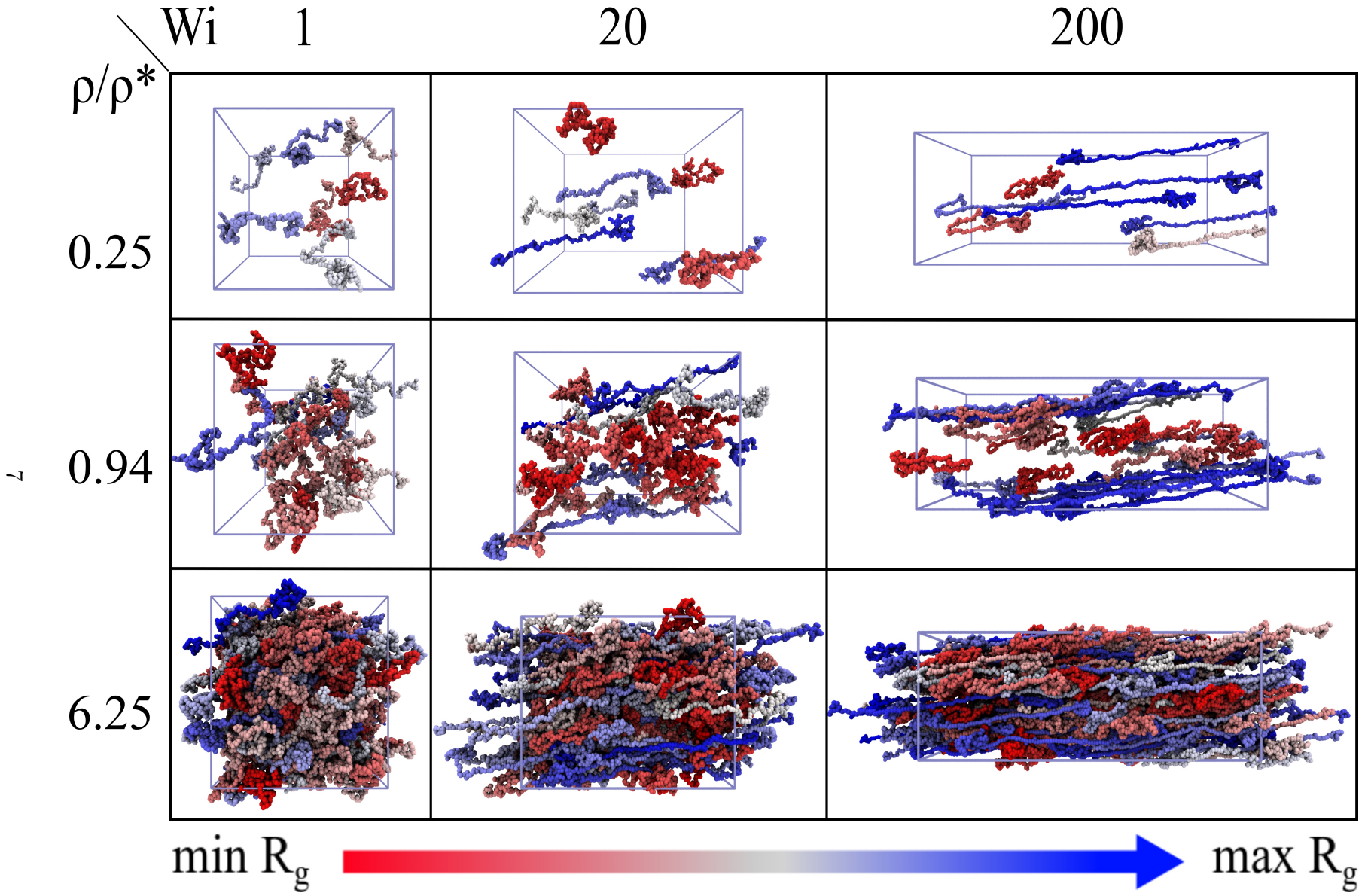

Figure S7. As Figure S3 for the monodisperse solution of SCNPs with high equilibrium asphericity $a_0 = 0.47$.

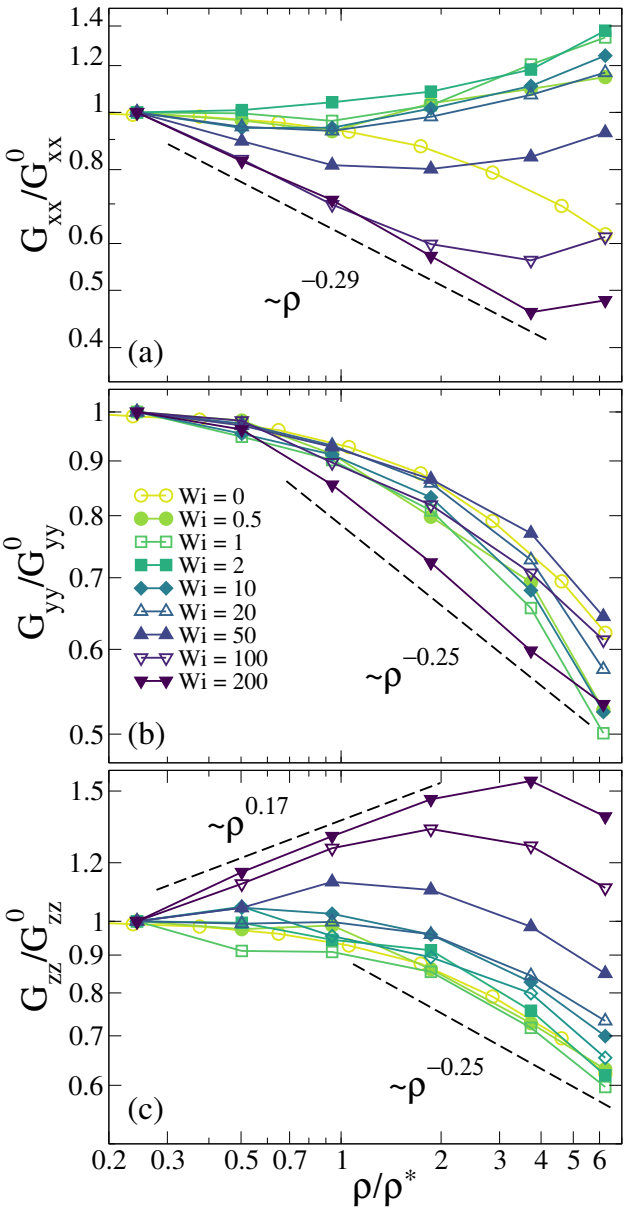

Figure S8. For the SCNPs in the polydisperse solutions, components of the gyration tensor vs. the concentration. Each data set corresponds to a fixed Weissenberg number (see legend) and is normalized by the value ($G^0_{\mu\mu}$) at its corresponding Wi and concentration $\rho/\rho^* = 0.25$. Dashed lines represent power laws.

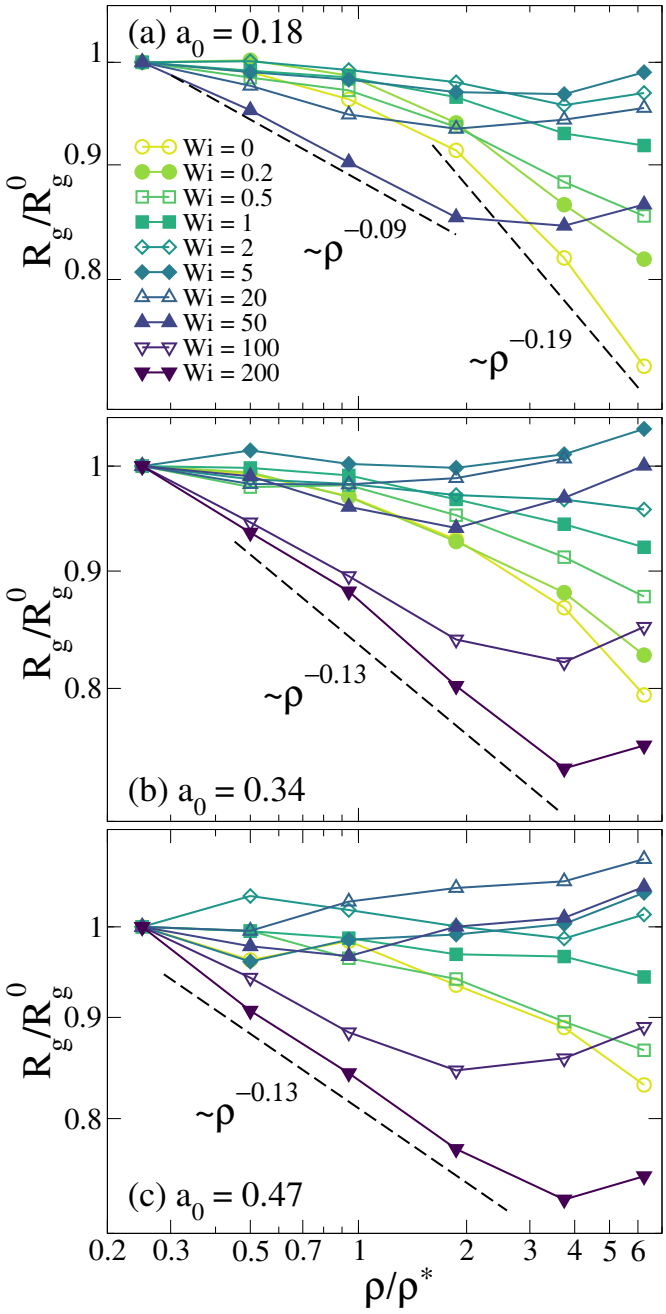

Figure S9. For the SCNPs in the monodisperse solutions, gyration radius vs. the concentration. Data are given for equilibrium asphericities $a_0 = 0.18$ (a), 0.34 (b) and 0.47 (c). Each data set corresponds to a fixed Weissenberg number (see legend) and is normalized by the value (R_{g0}) at its corresponding Wi and concentration $\rho/\rho^* = 0.25$. Dashed lines represent power laws.

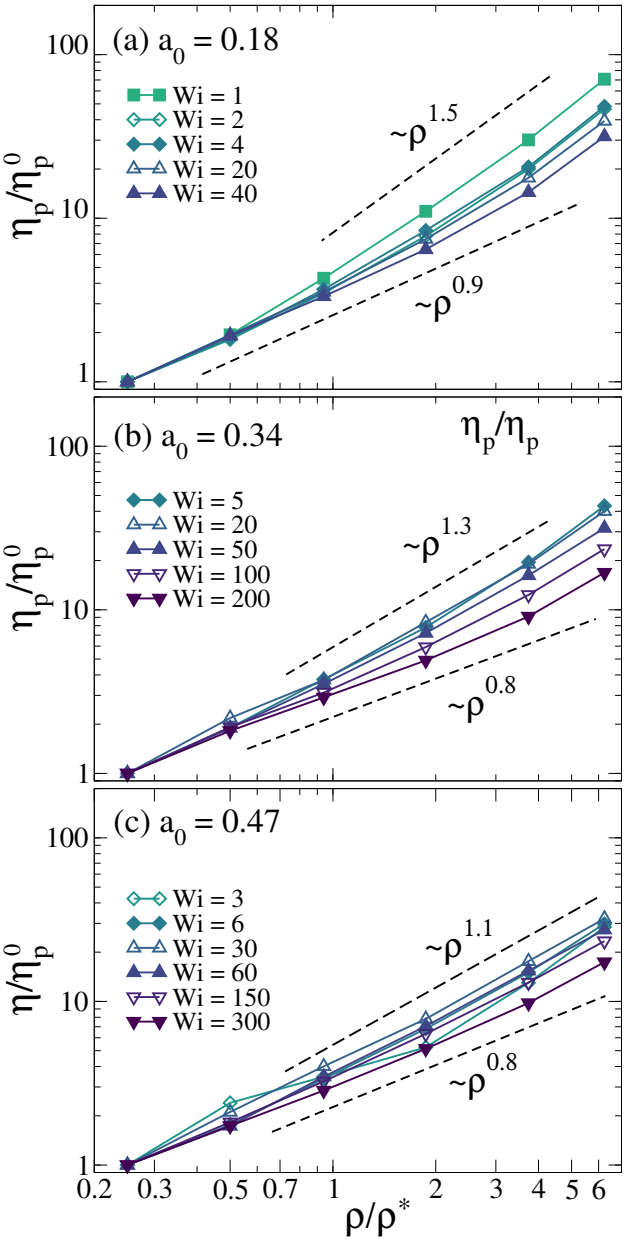

Figure S10. Polymer contribution to the viscosity vs. the concentration in monodisperse solutions of SCNPs with equilibrium asphericities $a_0 = 0.18$ (a), 0.34 (b) and 0.47 (c). Each data set corresponds to a value of the Weissenberg number (see legends) and is normalized by the value for that Wi at the lowest concentration $\rho/\rho^* = 0.25$.

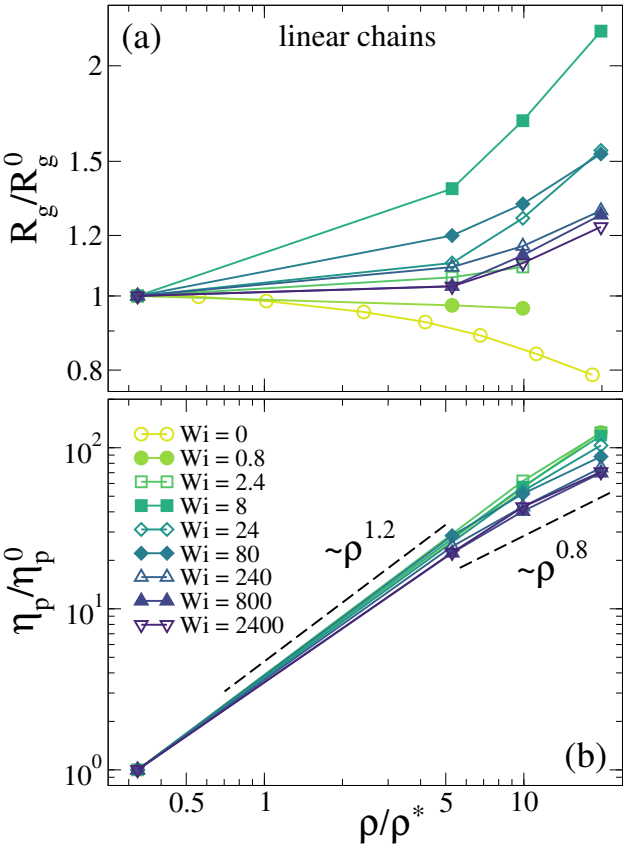

Figure S11. Radius of gyration (a) and polymer contribution to the viscosity (b) vs. the concentration, in solutions of linear chains (data are taken from Huang *et al.*, *Macromolecules* **43** (2010) 10107). Each data set corresponds to a fixed value of the Weissenberg number Wi (see legends), and is normalized by the value for that Wi at the lowest concentration $\rho/\rho^* \approx 0.3$. It must be noted that our definition of the overlap concentration is $\pi/6$ times the one used in the mentioned reference, so we have rescaled the data there by such a factor.

Movies: description

M1.mpg: Trajectory of the monodisperse solution of SCNPs with middle asphericity at $Wi = 200$ and $\rho/\rho^* = 3.74$.

M2.mpg: As M1.mpg for a slice perpendicular to the vorticity axis.

M3.mpg: As M1.mpg, highlighting the tumbling motion of a selected SCNP.