## Effects of generation number, spacer length and temperature on the structure and intramolecular dynamics of siloxane dendrimer melts: molecular dynamics simulations

## **Supporting Information**

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Figure S1. The radial density profile of the  $3^d$  generations for (a) s-dendrimers and (b) l-dendrimers. Red lines correspond to 600 K and blue ones to 300 K. Solid lines are for  $\rho_{in}$  and dashed lines show  $\rho_{out}$ . Black dashed dotted line demonstrates the radial density distribution calculated for single dendrimers in vacuum at 600K.



Figure S2. The radial density profile of the  $4^{th}$  generations for (a) s-dendrimers and (b) l-dendrimers. Red lines correspond to 600 K and blue ones to 300 K. Solid lines are for  $\rho_{in}$  and dashed lines show  $\rho_{out}$ . Black dashed dotted line demonstrates the radial density distribution calculated for single dendrimers in vacuum at 600K.



Figure S3. The radial density profile of the  $5^{th}$  generations for (a) s-dendrimers and (b) l-dendrimers. Red lines correspond to 600 K and blue ones to 300 K. Solid lines are for  $\rho_{in}$  and dashed lines show  $\rho_{out}$ . Black dashed dotted line demonstrates the radial density distribution calculated for single dendrimers in vacuum at 600K.



Figure S4. Log-log universal scaling plots for (a) good and (b) theta solvents regimes. S=1 and S=2 for s- and ldendrimers, respectively; N is the number of Si-O-Si segments and b is the average length of this segment. Red symbols correspond to 600 K and blue ones to 300 K. Filled symbols correspond to melts and open symbols to isolated dendrimers. Black lines show the slopes of 1/5 and 1/4 theoretically predicted for good and theta solvents, respectively.



Figure S5. The examples of the angular autocorrelation function of one of the terminal groups of the generation-3 and 6 for s- and l-dendrimers. The red line shows exponential fitting. The green line indicates the value of 1/e.



Figure S6. The average relaxation times and dispersions for angular (O) and radial (R) motions for 300 K (blue line) and 600 K (red line) for the G4 s-dendrimer (left column) and l-dendrimer (right column). The solid lines are for dendrimers in melt and dashed lines are for isolated dendrimers.



Figure S7. The average relaxation times and dispersions for angular (O) and radial (R) motions for 300 K (blue line) and 600 K (red line) for the G5 s-dendrimer (left column) and l-dendrimer (right column). The solid lines are for dendrimers in melt and dashed lines are for isolated dendrimers.