Molecular Dynamics of Variegated Polyamide Dendrimers

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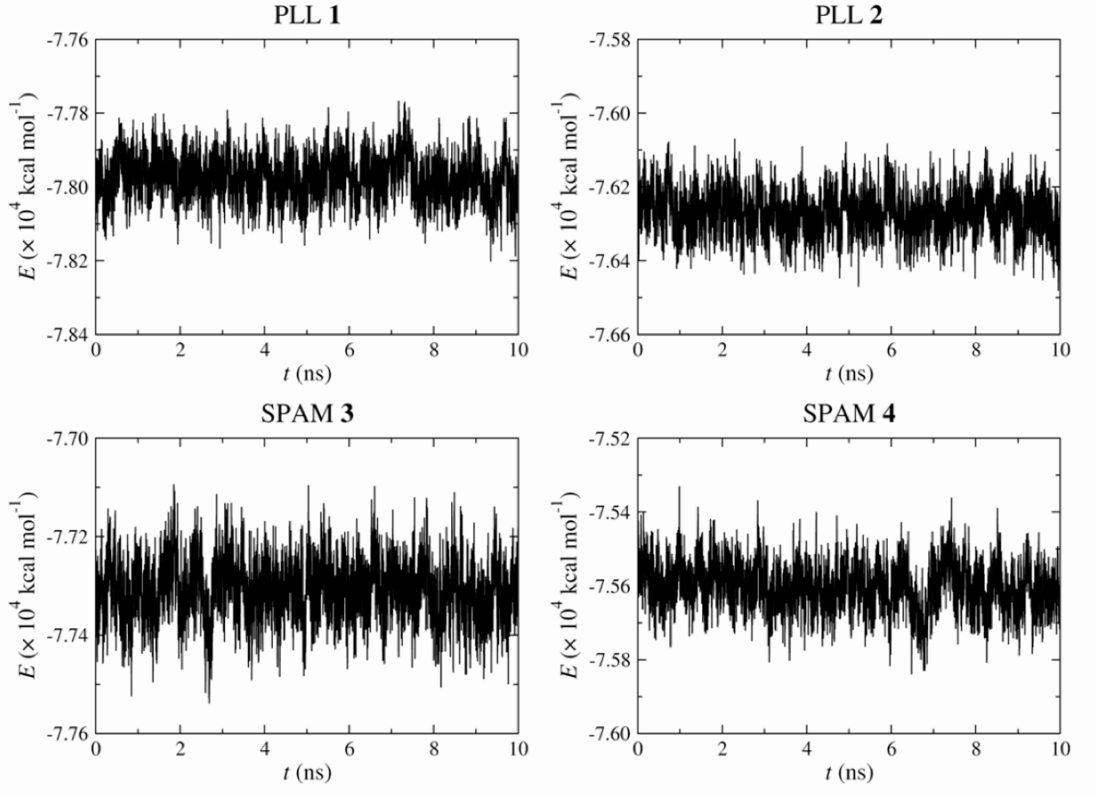

Figure S1: Simulation energies of the dendrimers **1**-**4** (conformer 3) during production molecular dynamics. Energies shown are the "TOTAL3" energy computed by NAMD, a sum of potential and kinetic energy with reduced short-time fluctuations.

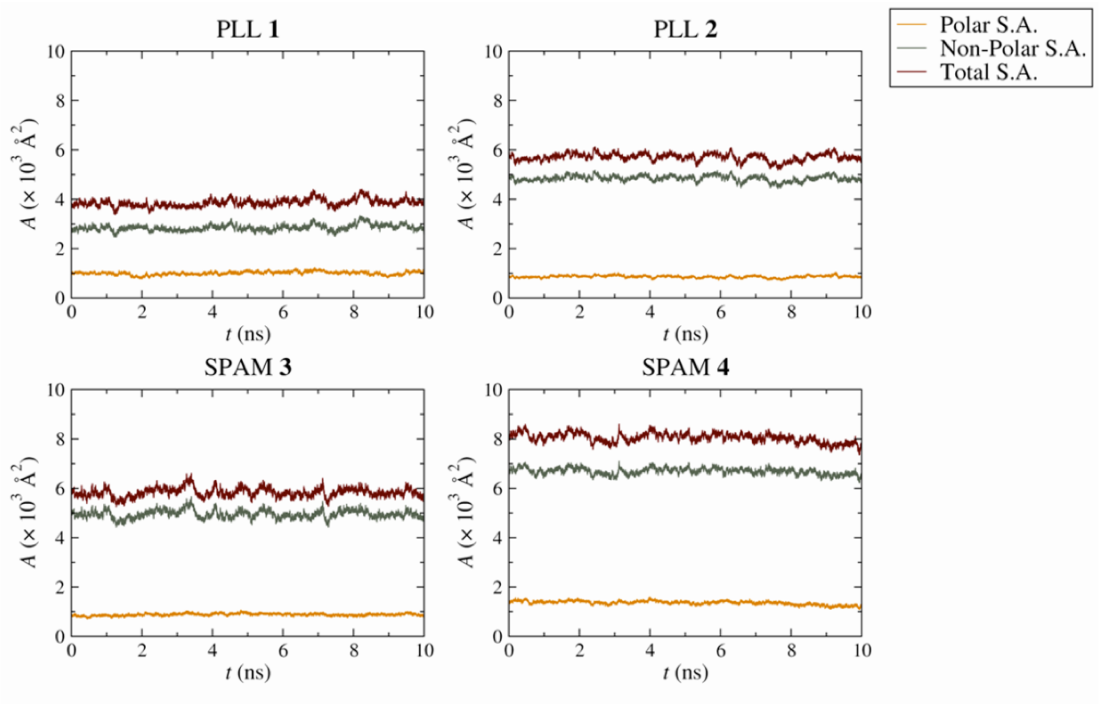

Figure S2: Solvent-accessible surface areas of the dendrimers **1**-**4** (conformer 3) during production molecular dynamics. Polar surface areas are contributed by polar heavy atoms (i.e., nitrogen, oxygen); non-polar surface areas are contributed by carbon atoms.

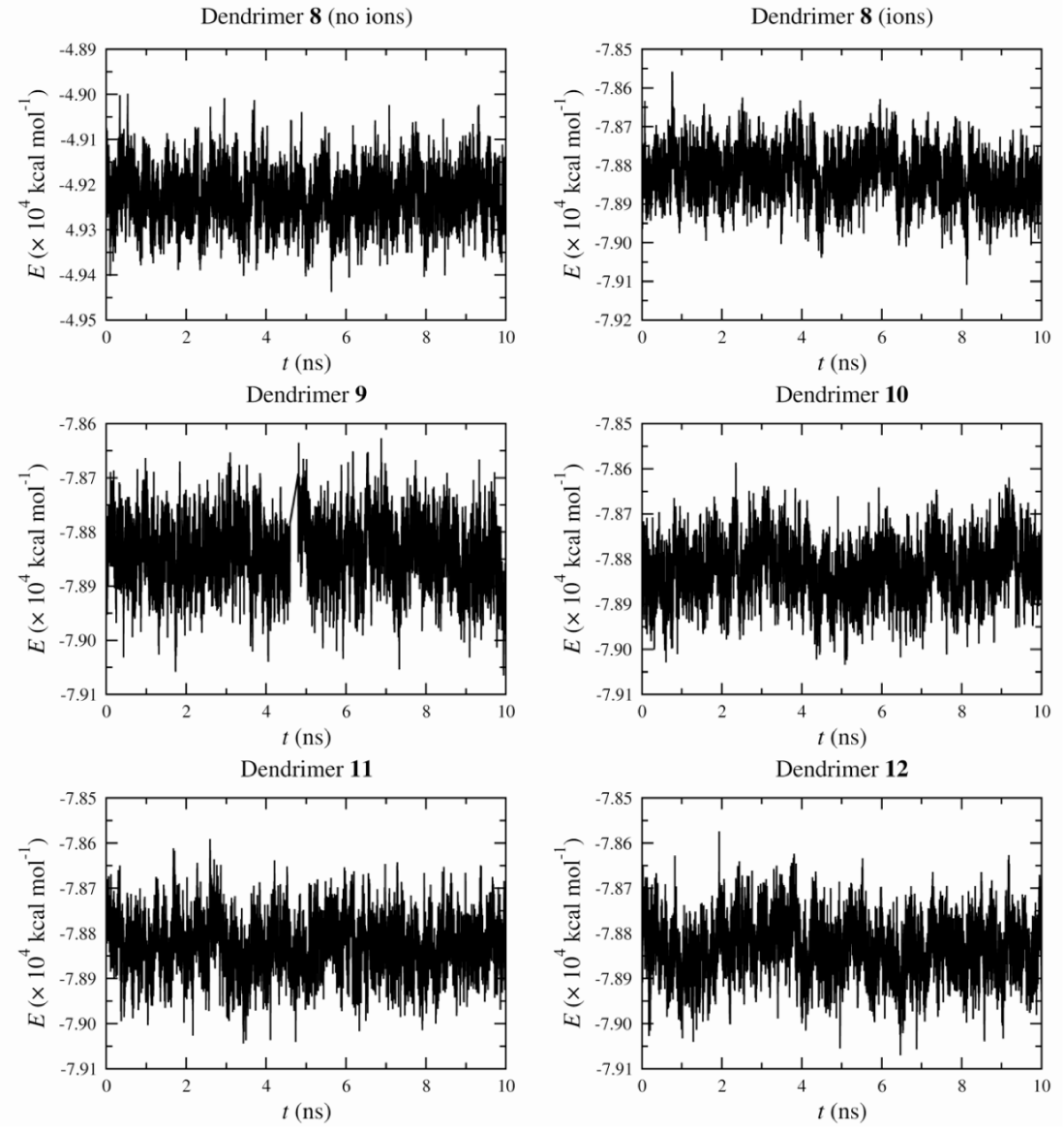

Figure S3: Instantaneous total simulation energies (NAMD TOTAL3) for the variegated SPAM dendrimers **8** – **12**, capped with ammonium and carboxylate groups. **8** is variegated with pattern I, **9** with pattern II, and so on.

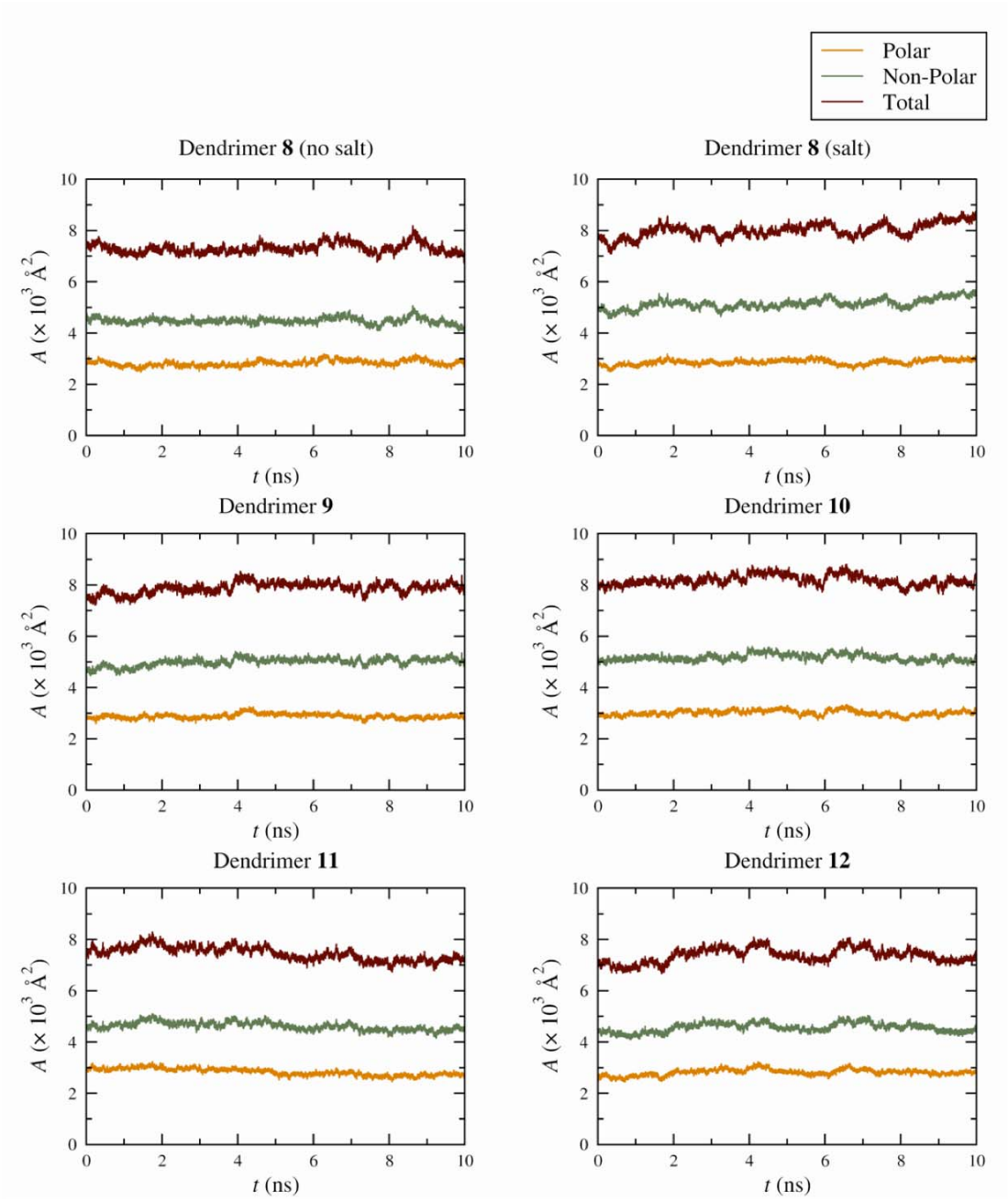

Figure S4: Instantaneous solvent-accessible surface areas for the variegated SPAM dendrimers **8** – **12**, capped with ammonium and carboxylate groups. **8** is variegated with pattern I, **9** with pattern II, and so on. Surface areas for polar and non-polar atoms, and the total solvent-accessible surface area, are shown for each dendrimer. Polar surface areas are contributed by polar heavy atoms (i.e., nitrogen, oxygen); non-polar surface areas are contributed by carbon atoms.

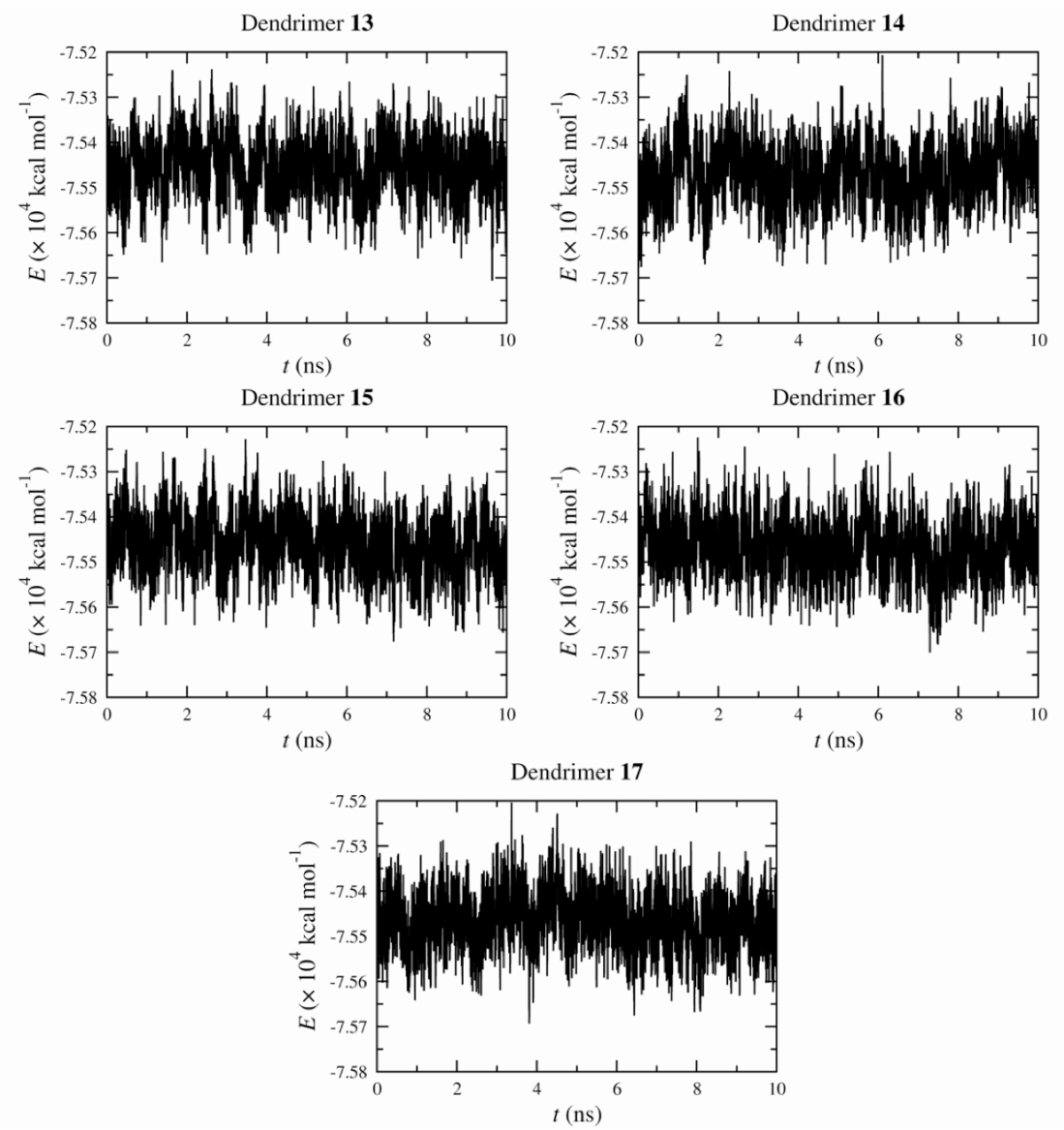

Figure S5: Instantaneous total simulation energies (NAMD TOTAL3) for the variegated SPAM dendrimers **13** – **17**, capped with ammonium and alcohol groups. **13** is variegated with pattern I, **14** with pattern II, and so on.

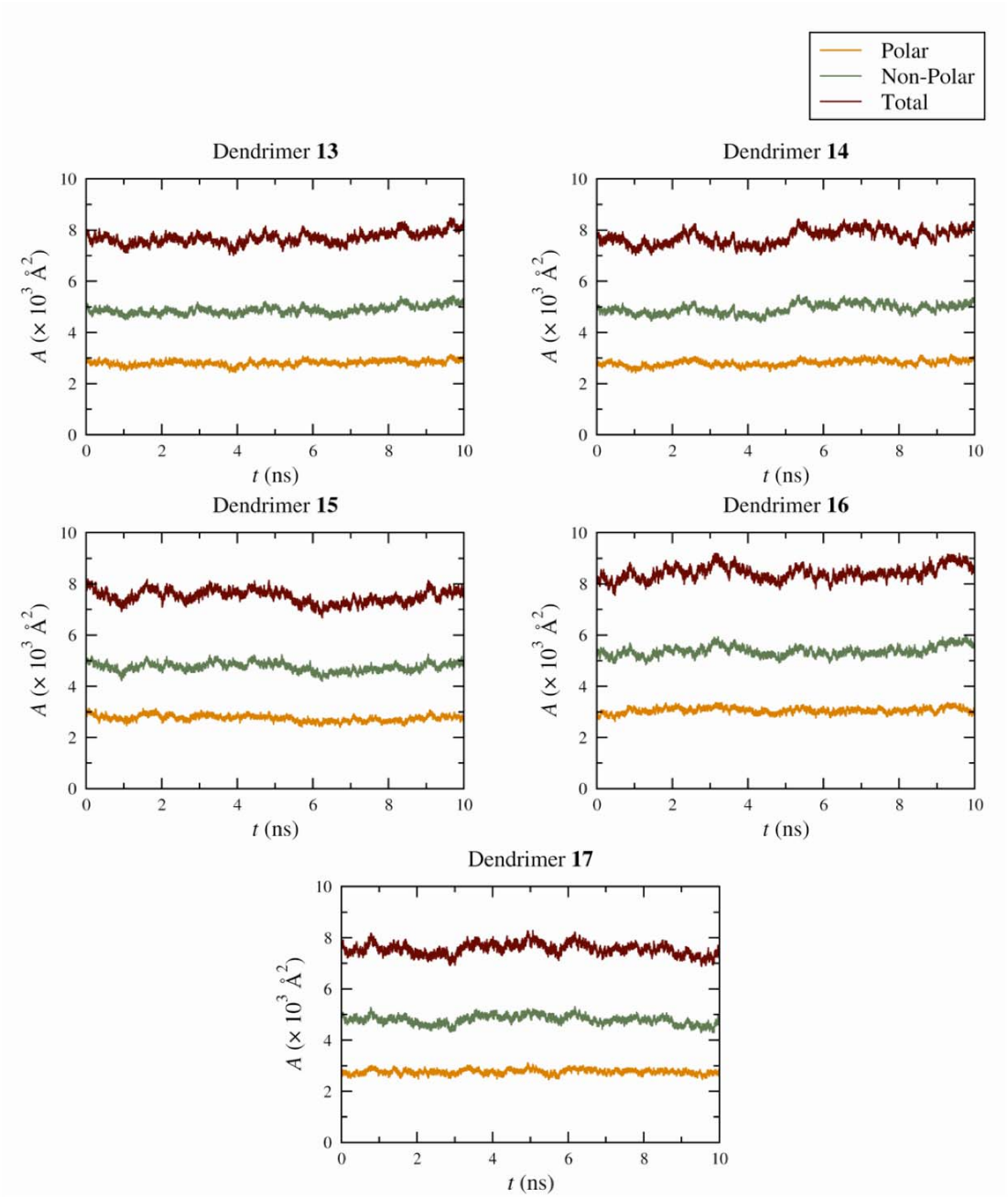

Figure S6: Instantaneous solvent-accessible surface areas for the variegated SPAM dendrimers **13** – **17**, capped with ammonium and alcohol groups. **13** is variegated with pattern I, **14** with pattern II, and so on. Surface areas for polar and non-polar atoms, and the total solvent-accessible surface area, are shown for each dendrimer. Polar surface areas are contributed by polar heavy atoms (i.e., nitrogen, oxygen); non-polar surface areas are contributed by carbon atoms.

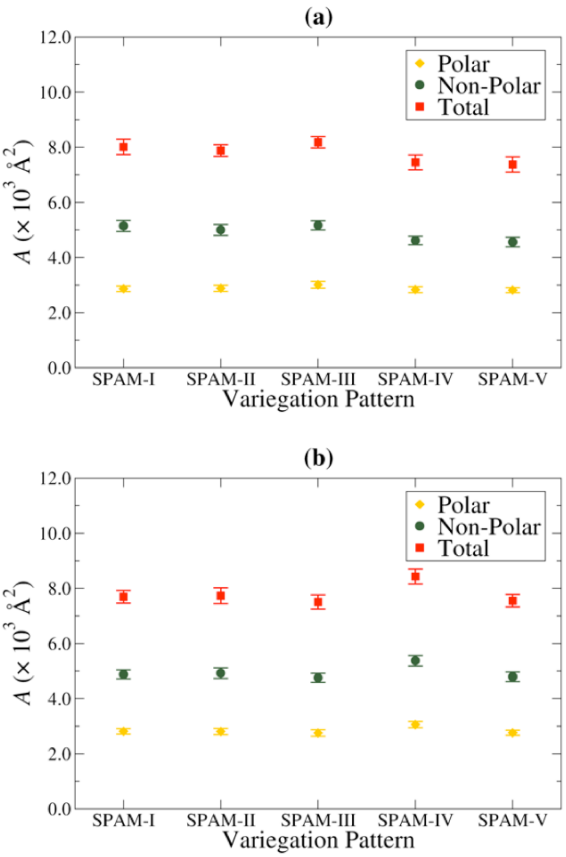

Figure S7: Polar, non-polar and total solvent-accessible surface areas of (a) the ammonium/carboxylate capped dendrimers **8** – **12**, and (b) the ammonium/alcohol capped dendrimers **13** – **17**. Polar surface areas are contributed by polar heavy atoms (i.e., nitrogen, oxygen); non-polar surface areas are contributed by carbon atoms.

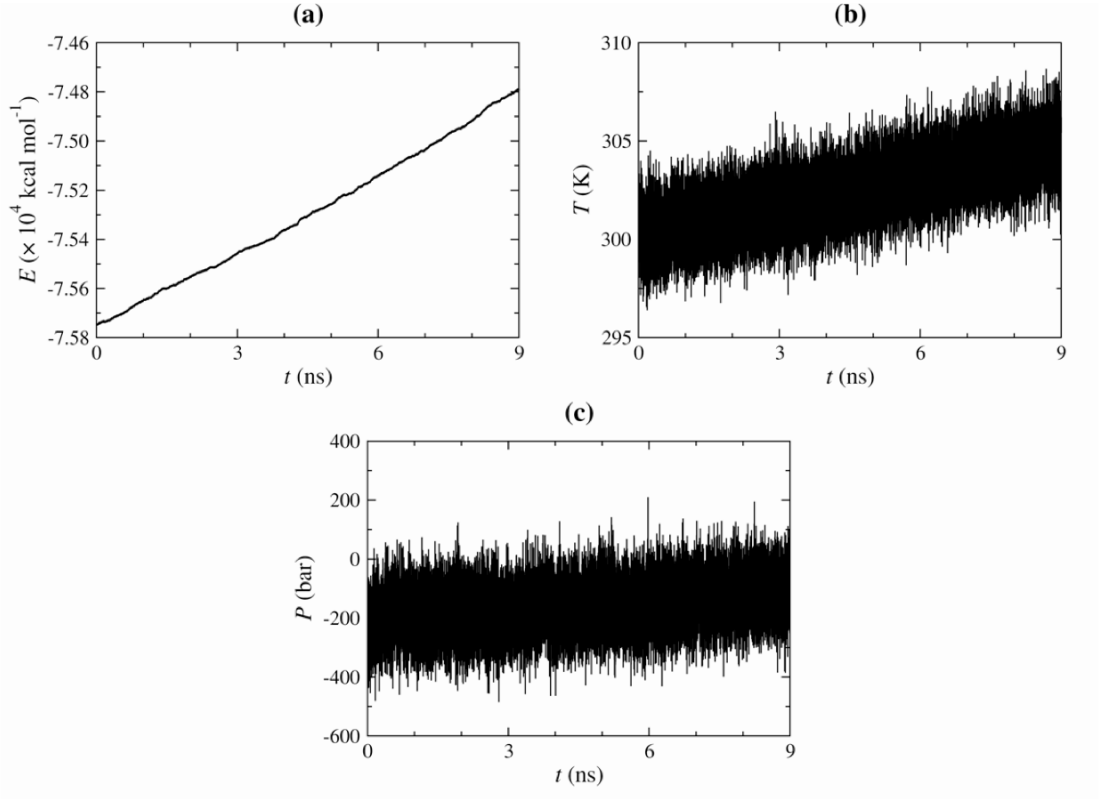

Figure S8: Behaviour of the protonated SPAM dendrimer (conformer 1) in an NVE ensemble over 9 ns. (a) Total system energy. (b) System temperature. (c) System pressure. The system shows a modest increase in energy, temperature and pressure due to integration errors.

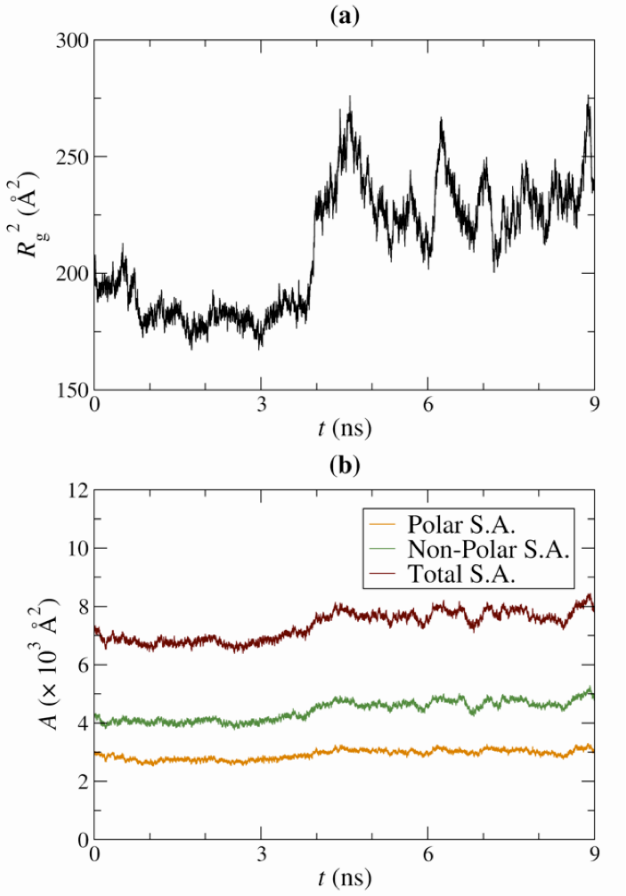

Figure S9: Properties of the protonated SPAM dendrimer (conformer 1) under an NVE ensemble. (a) The instantaneous mean-squared radius of gyration. (b) The solvent-accessible surface areas of polar (nitrogen, oxygen), non-polar (carbon) and all heavy atoms. During the course of this simulation, the dendrimer equilibrates and expands from a compressed starting geometry to give a mean-squared radius of gyration and surface areas that are in good agreement with the NPT simulations.

Table S1: Comparison of the mean-squared radius of gyration and mean asphericity of the protonated SPAM dendrimer (conformer 1) under the NPT and NVE ensembles. Values in brackets are standard deviations.

Property	NPT ensemble	NVE ensemble
Mean-squared radius of gyration, R_g^2 (Å^2)	218.6 (16.8)	211.0 (26.1)
Asphericity, δ	0.101 (0.040)	0.077 (0.035)