

## Supplementary Material

# Self-assembly Behavior of Amphiphilic Janus Dendrimers in Water: A Combined Experimental and Coarse-Grained Molecular Dynamics Simulation Approach

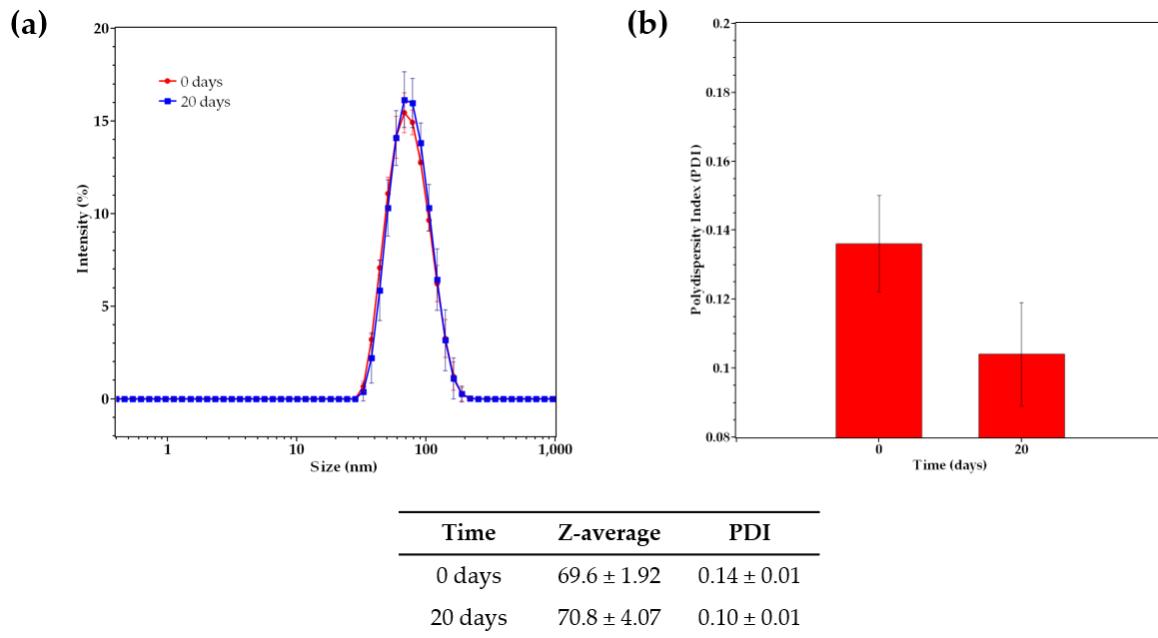
Mariana E. Elizondo-García <sup>1,\*</sup>, Valeria Márquez-Miranda <sup>2</sup>, Ingrid Araya-Durán <sup>2</sup>, Jesús A. Valencia-Gallegos <sup>1,\*</sup> and Fernando D. González-Nilo <sup>2,3</sup>

<sup>1</sup> Escuela de Ingeniería y Ciencias, Tecnológico de Monterrey, Av. Eugenio Garza Sada 2501 Sur, Monterrey 64849, Mexico

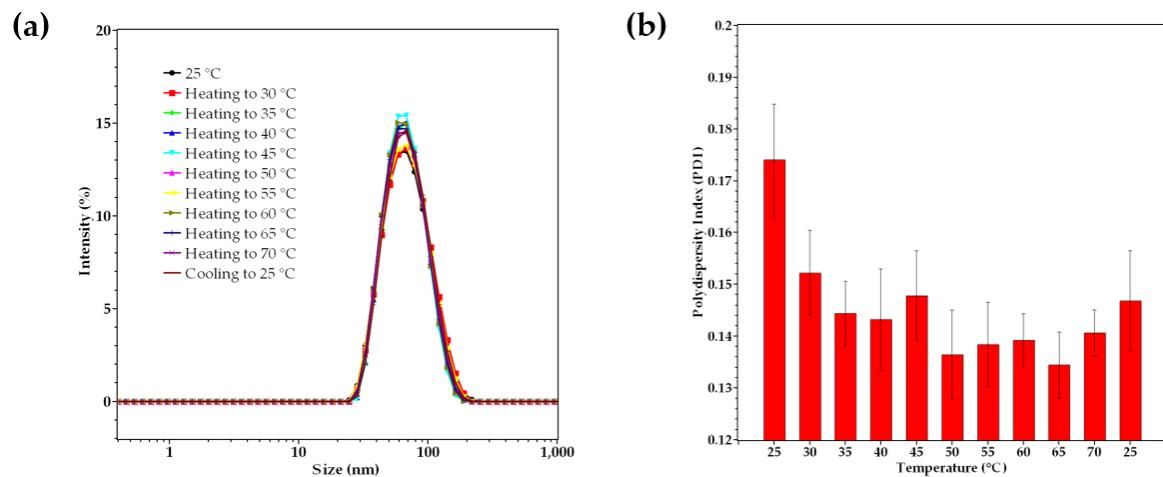
<sup>2</sup> Center for Bioinformatics and Integrative Biology (CBIB), Facultad de Ciencias Biológicas, Universidad Andrés Bello, Av. República 330, Santiago 8370186, Chile; valeria.marquez.m@gmail.com (V.M.M.); ingrid.araya.duran@gmail.com (I.A.D.); fernando.gonzalez@unab.cl (F.D.G.N.).

<sup>3</sup> Centro Interdisciplinario de Neurociencia de Valparaíso, Facultad de Ciencias, Universidad de Valparaíso, Gran Bretaña 1111, Playa Ancha, Valparaíso 2360102, Chile

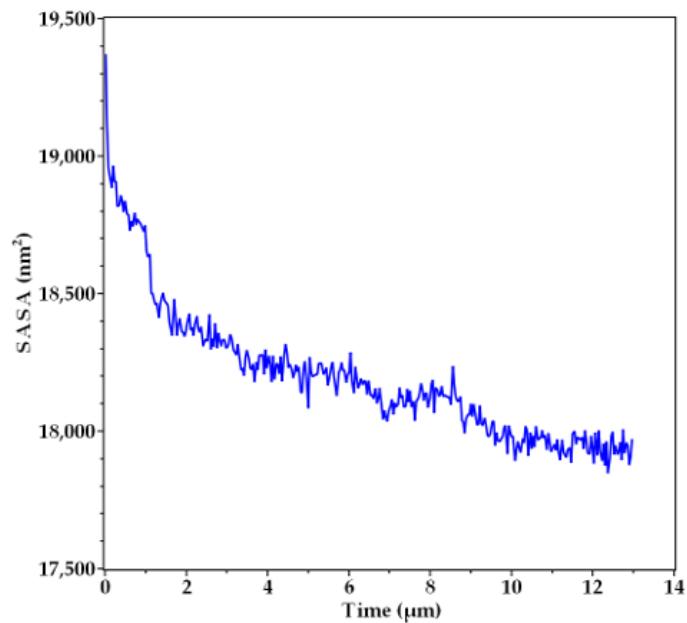
\* Correspondence: mariana.elizndo@gmail.com (M.E.E.G); valencia@itesm.mx (J.A.V.G);  
Tel.: +52-818-358-2000 (ext. 4511) (J.A.V.G)



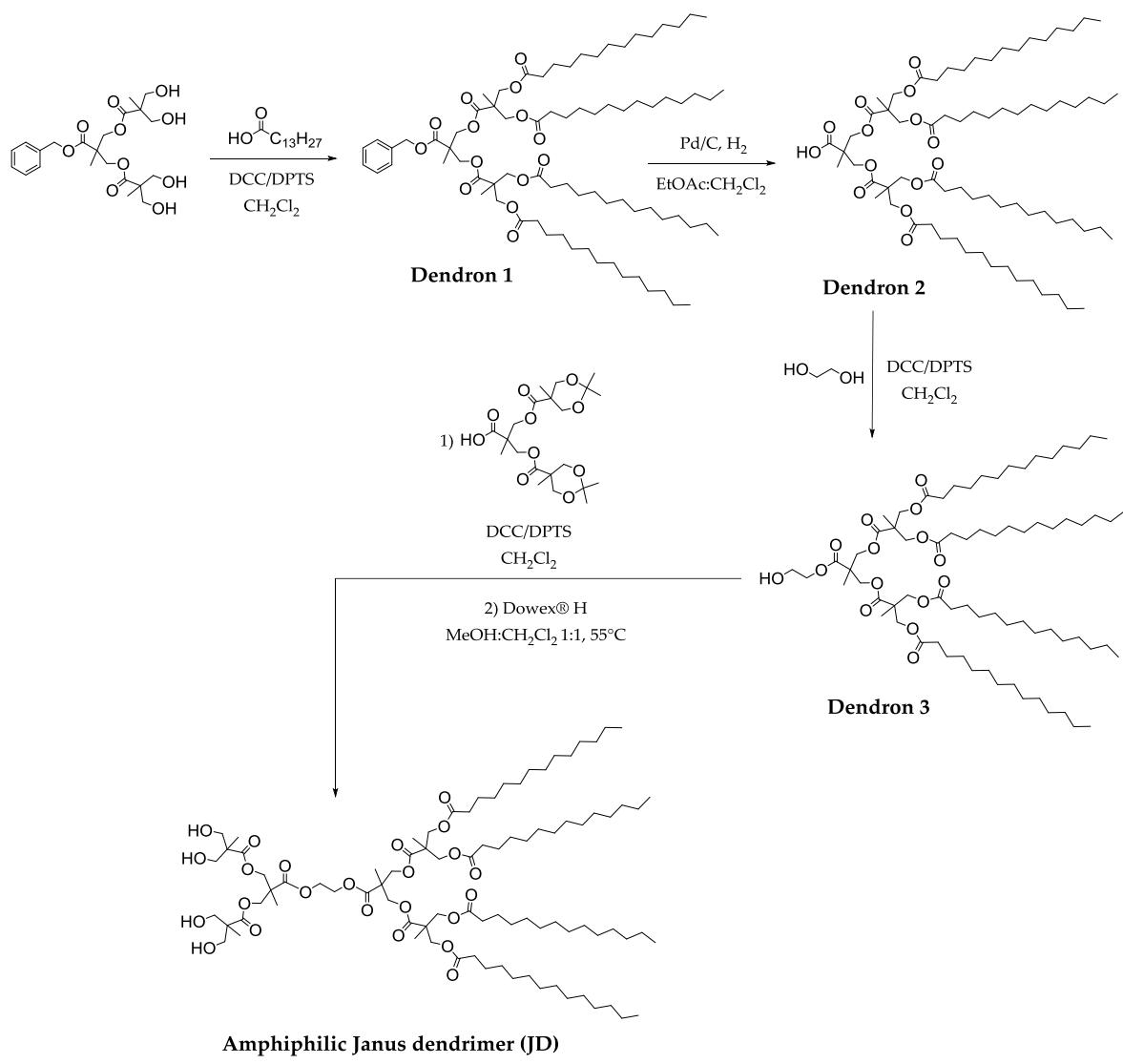
**Figure S1.** Time stability of small assemblies from JD. (a) Size distribution by intensity and (b) PDI variation (by DLS).



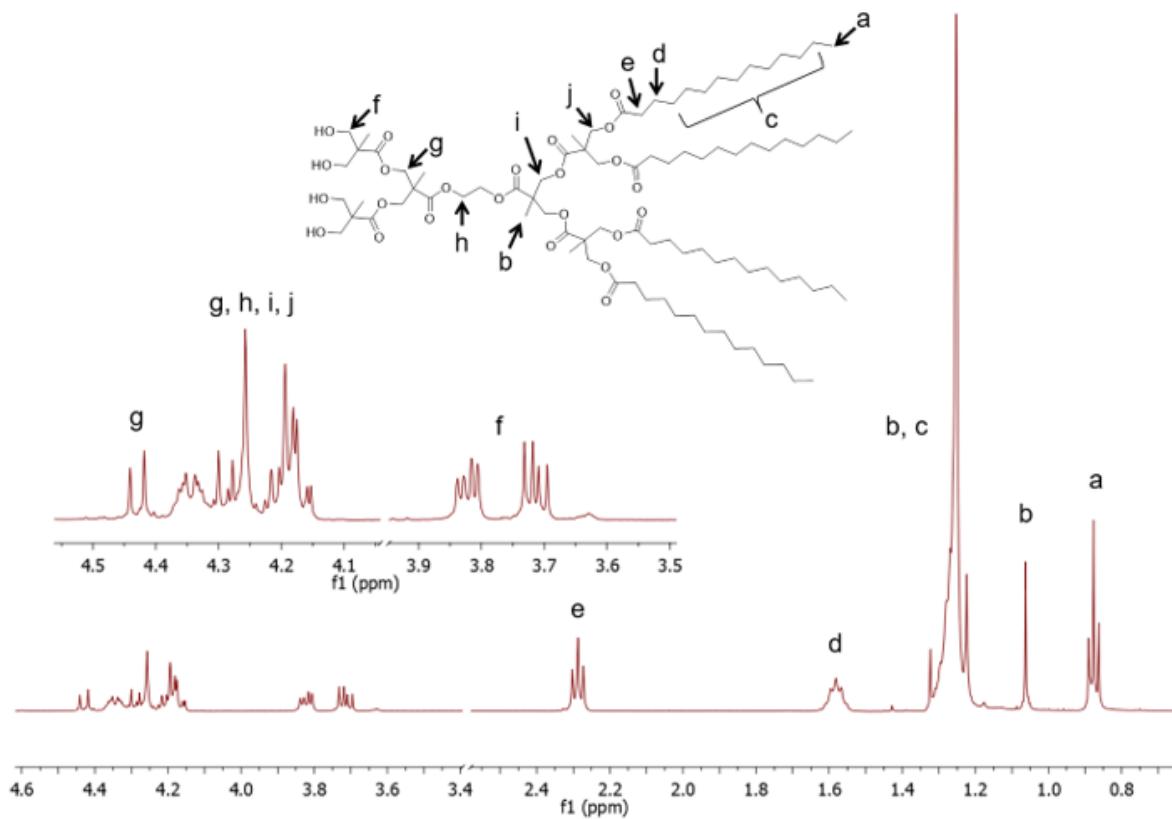
**Figure S2.** Temperature stability of small assemblies from JD. (a) Size distribution by intensity and (b) PDI variation (by DLS).



**Figure S3.** Solvent accessible surface area (SASA) of the dendrimers during the simulation.



**Figure S4.** Reaction scheme.



**Figure S5.** <sup>1</sup>H-NMR spectra (500 MHz, CDCl<sub>3</sub>) of JD and peak assignments.