Interaction studies reveal specific recognition of an anti-inflammatory polyphosphorhydrazone dendrimer by human monocytes

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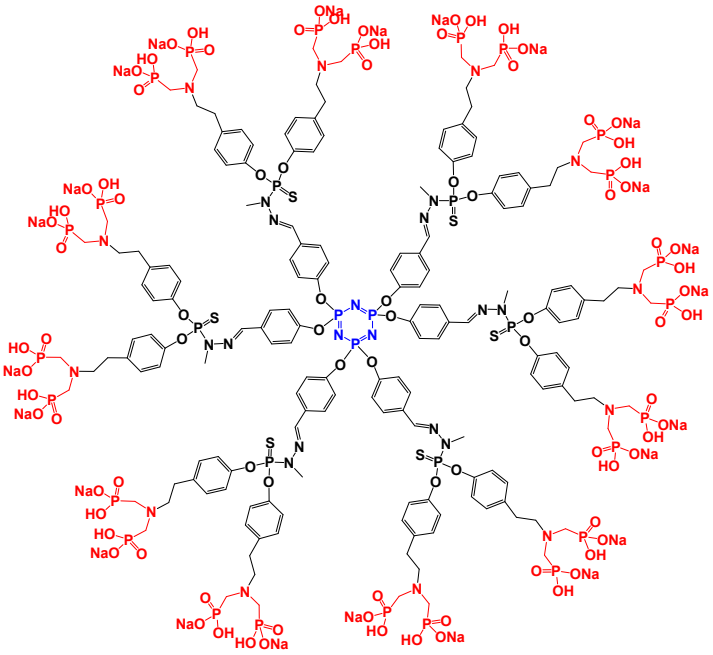
(a)



(b)

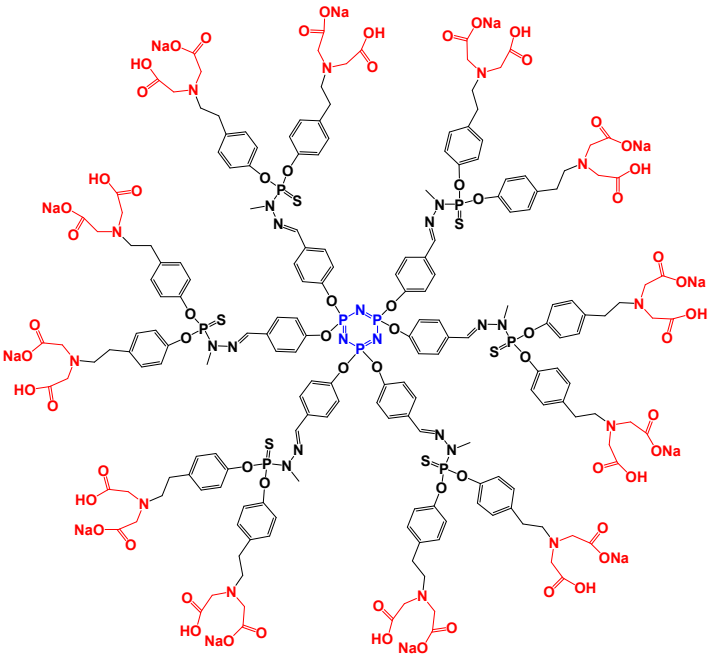


Fig. S1 Two-dimensional structures of (a) dendrimer **1** (ABP) and (b) dendrimer **2** (ABC).

Table S1

Main transition calorimetric data[a] for MLV suspensions of pure DPPC (30 mM) alone, and with dendrimers **1**, **2**, **6** or **9** (3 mM).

	Scan number	T_m (°C)	ΔH[b]
MLV alone	1st	40.99	-8.87
	4th	41.04	-8.96
MLV + **1**	1st	41.03	-7.48
	4th	41.05	-7.48
MLV + **6**	1st	41.01	-7.24
	4th	41.02	-7.38
MLV + **2**	1st	41.06	-7.31
	4th	41.10	-7.47
MLV + **9**	1st	40.90	-7.33
	4th	40.97	-7.47

[a] Values are given for heating cycles. Cooling cycles gave comparable absolute values. [b] ΔH: transition enthalpy normalized per mole of DPPC. Unit is $kcal.mol^{-1}$.

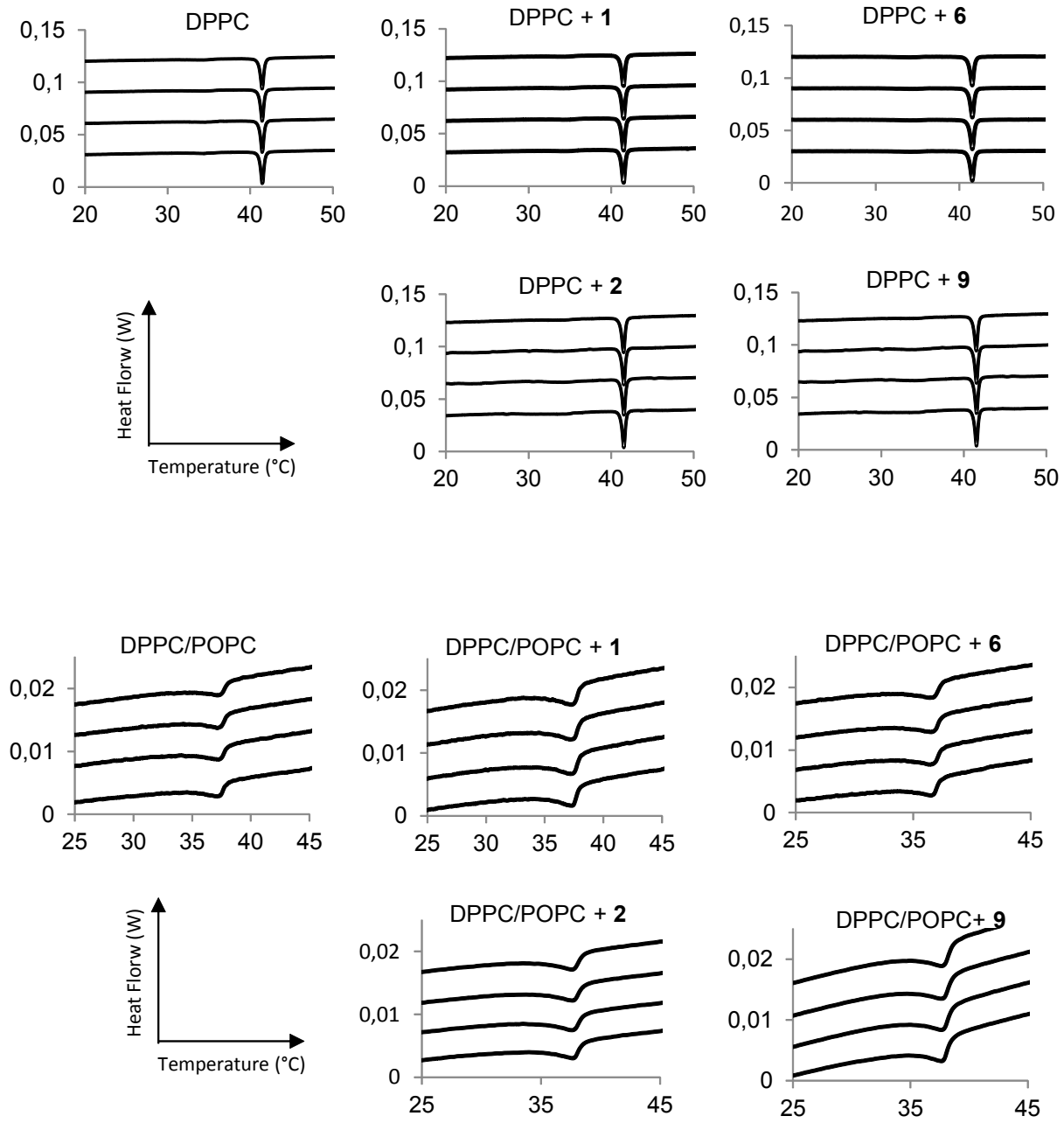


Fig. S2 DSC scans for pure DPPC and DPPC/POPC (30 mM) MLV suspensions in the presence of dendrimers **1**, **2**, **6** or **9** (3 mM).

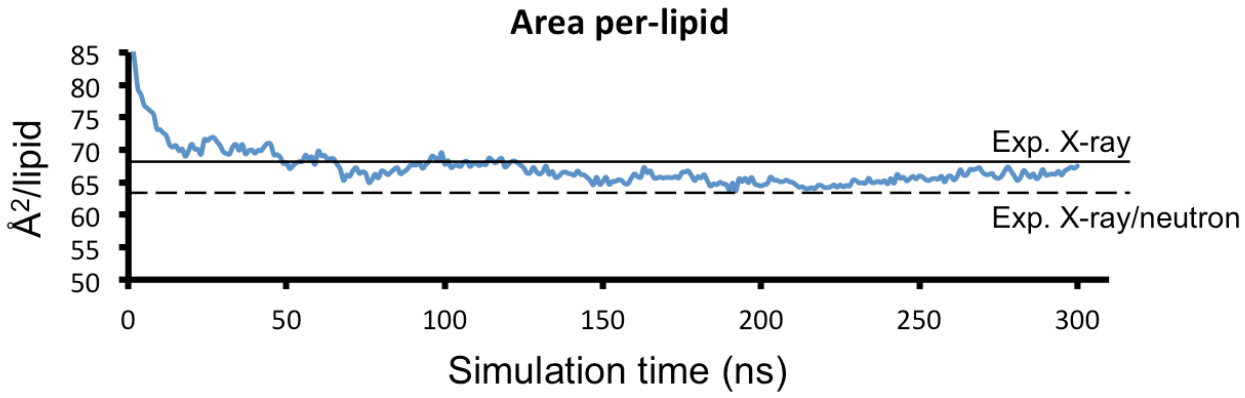


Fig. S3 Area per lipid for the POPC model extracted from the MD simulation as a function of simulation time. The simulation data (blue) is in good agreement with the experimental results (dotted and solid black lines).[1,2]

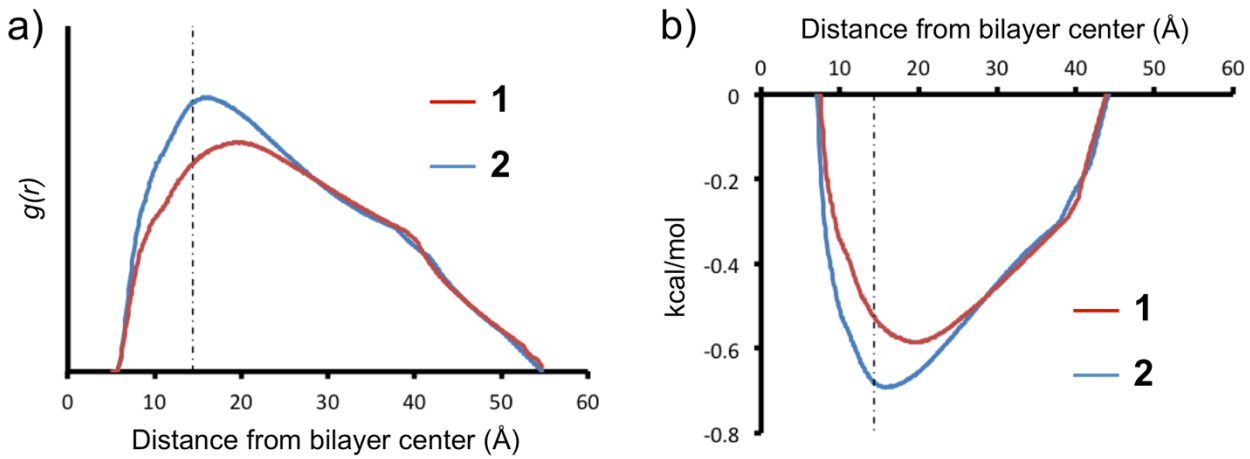


Fig. S4 Dendrimers absorption onto the POPC membrane. (a) Radial distribution functions of the centres of mass of dendrimers **1** (red) and **2** (blue) calculated respect to the lipid bilayer centre (origin of the *x* axis). (b) Free energy of absorption (ΔA) extracted from the *g(r)* data as A=-kT ln(*g(r)*).[3–5] The dotted lines identify the lipid bilayer surface (centres of mass of the lipid heads).

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