Exploring the interactions of ruthenium(II) carbosilane metallodendrimers and precursors with model cell membranes through a dual Spin-Label Spin-Probe technique using EPR

Riccardo Carloni^{1†,} Natalia Sanz del Olmo^{234†}, Paula Ortega²³⁴, Alberto Fattori¹, Rafael Gómez²³⁴, Maria Francesca Ottaviani¹, Sandra García-Gallego ²³⁴, Michela Cangiotti¹* and F. Javier de la Mata²³⁴*

^aDepartment of Pure and Applied Sciences, University of Urbino "Carlo Bo", Urbino, Italy.

^bDepartment of Organic and Inorganic Chemistry, and Research Institute in Chemistry Andrés M. del Río" (IQAR), University of Alcalá, Madrid, Spain;

^cNetworking Research Center on Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), Spain.

^dInstitute Ramón y Cajal for Health Research (IRYCIS), Spain.

Figures



Figure S1. ¹H- and ¹³C{¹H}-NMR spectra of compound 1 in CDCl₃.



Figure S2. TOCSY 1D spectrum of compound 1 in CDCl₃.



Figure S3. ¹H-NMR spectrum of compound 3 in CD₃OD.



Figure S4. ¹H-NMR spectrum of compound 5 in CD₃OD.



Figure S5. FT-IR spectra of precursor 4-isothiocyanateTEMPO (top) and compound **3** (bottom) in KBr.



Figure S6. Examples of experimental and computed spectra of labelled dendrimers in the absence and presence of model membranes. Experimental and computed spectra of G₁-PyT, only constituted by the Free component (A). Experimental and computed Interacting component, obtained after subtraction of the Free component, of: (B) G₁-PyT+CTAB; (C) G₁-PyT+LEC; (D) G₁-RuT+LEC. The spectra are normalized in height.



Figure S7. Examples of experimental and computed spectra of non-labelled dendrimers in the absence and presence of model membranes. Experimental and computed spectra of CAT12 in G₂-PyN, only constituted by a free component (A). Examples of computations of the interacting component for CAT12 in: LEC (B); and G₂-PyN+LEC (C).



Figure S8: A_{zz} values obtained by computing the Free and the Interacting components for CTAB for homofunctional dendrimers G_n -Py.