Supporting Information

The Effect of Size, Surface Charge and Hydrophobicity of Poly(amidoamine) Dendrimers on Their Skin Penetration

*Yang Yang[1], Suhair Sunoqrot[1], Chelsea Stowell[1], Jingli Ji[1], Chan-Woo Lee[2], Jin Woong Kim[3], Seema A. Khan[4], and Seungpyo Hong[1]**

[1]Department of Biopharmaceutical Sciences, College of Pharmacy, University of Illinois, Chicago, IL 60612

[2]Durae Co. Research and Development Center, Gunpo, Gyeonggi-do, Republich of Korea

[3]Department of Applied Chemistry, Hanyang University, Ansan, Gyeonggi-do, Republic of Korea

[4]Robert H. Lurie Comprehensive Cancer Center, Northwestern University, Chicago, IL 60611

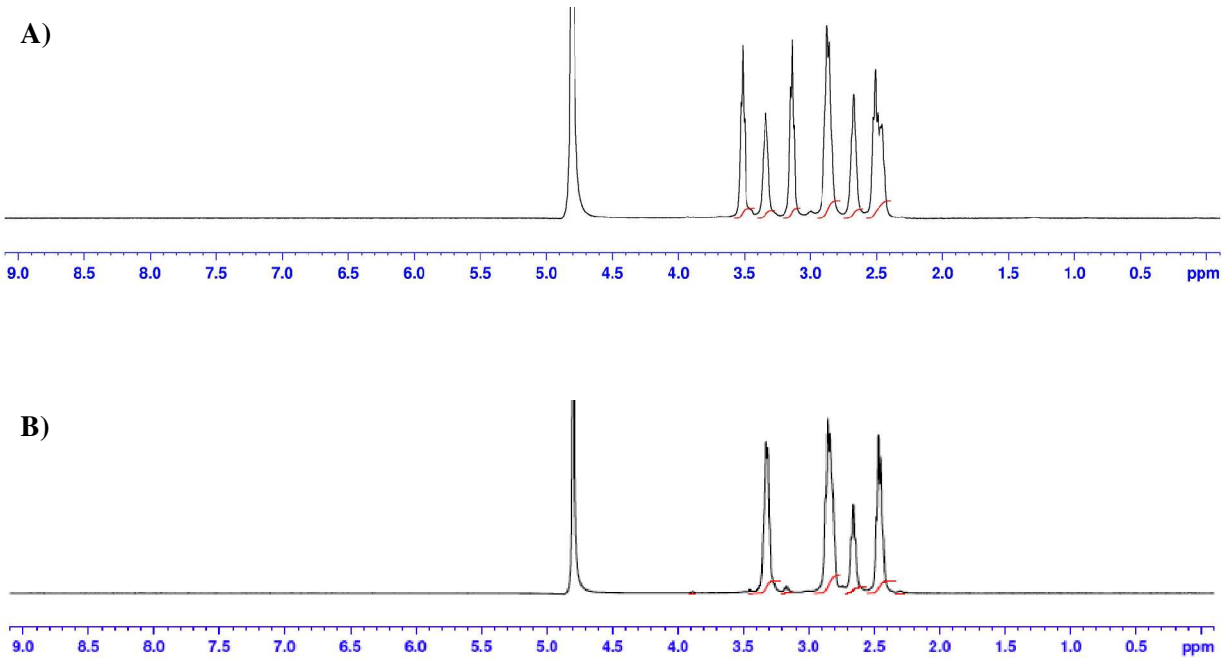

Figure S1. ^{1}H NMR spectra of the starting materials G2-NH_2 and G4-NH_2. A) Starting G2 PAMAM dendrimer with primary amine end groups (G2-NH_2) and B) Starting G4 PAMAM dendrimer with primary amine end groups (G4-NH_2).

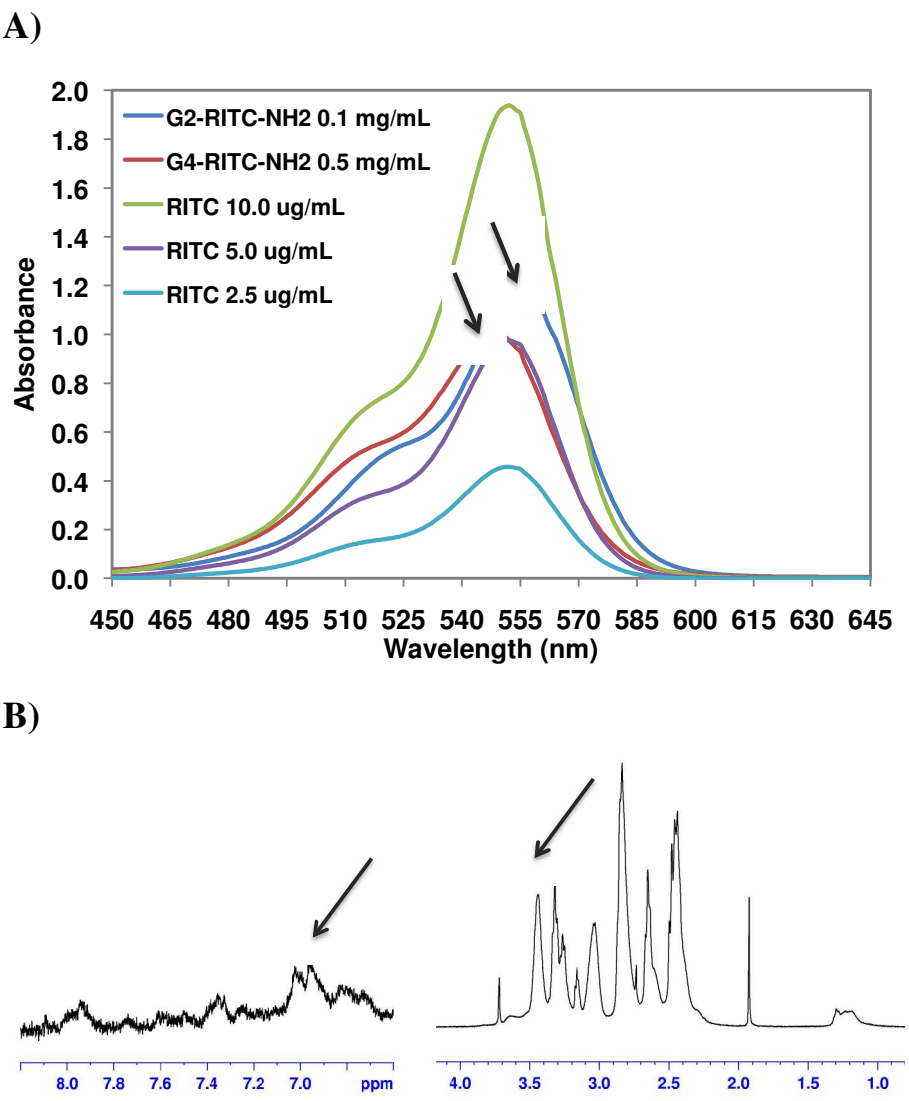

Figure S2. Characterization of G2-RITC-NH_2 and G4-RITC-NH_2 using A) UV/Vis and B) ^{1}H NMR spectroscopy.

The ratio of dendrimer to RITC was calculated based on UV spectra of RITC standards. RITC exhibits a maximum absorption peak at 554 nm, which was shifted after conjugation to dendrimer (see arrows, peak shifted to 555 nm for G2-RITC-NH_2, and 548 nm for G4-RITC-NH_2). Serially diluted RITC (2.5, 5, and 10 µg/mL) solutions in 1:1 DMSO/H_2O were prepared and used to plot the standard curve for the quantification of the number of RITC on the dendrimer conjugates. The ratio was 1:1 for both G2-RITC-NH_2 and G4-RITC-NH_2. The integration values of the characteristic peaks from ^{1}H NMR measurements (see arrows, 3.442 ppm for G2 dendrimer, 6.963 ppm for RITC) also revealed the ratio of approximately 1:1.3.

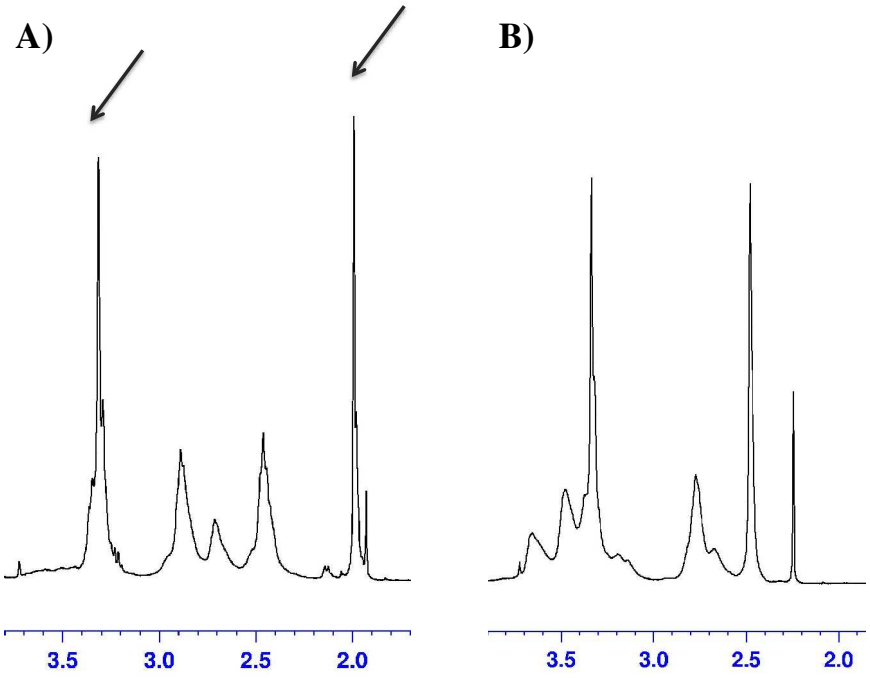

Figure S3. ^{1}H NMR spectra of A) G2-RITC-Ac and B) G2-RITC-COOH.

The degree of acetylation was determined by comparing the integration values of the characteristic peaks of G2 dendrimer at 3.31 ppm and acetyl group at 2.06 ppm (see arrows). The measured ratio revealed that 94.3% of the primary amine groups were acetylated. The shape changes of characteristic peaks of dendrimer after carboxylation demonstrate that the surface modification was successful.

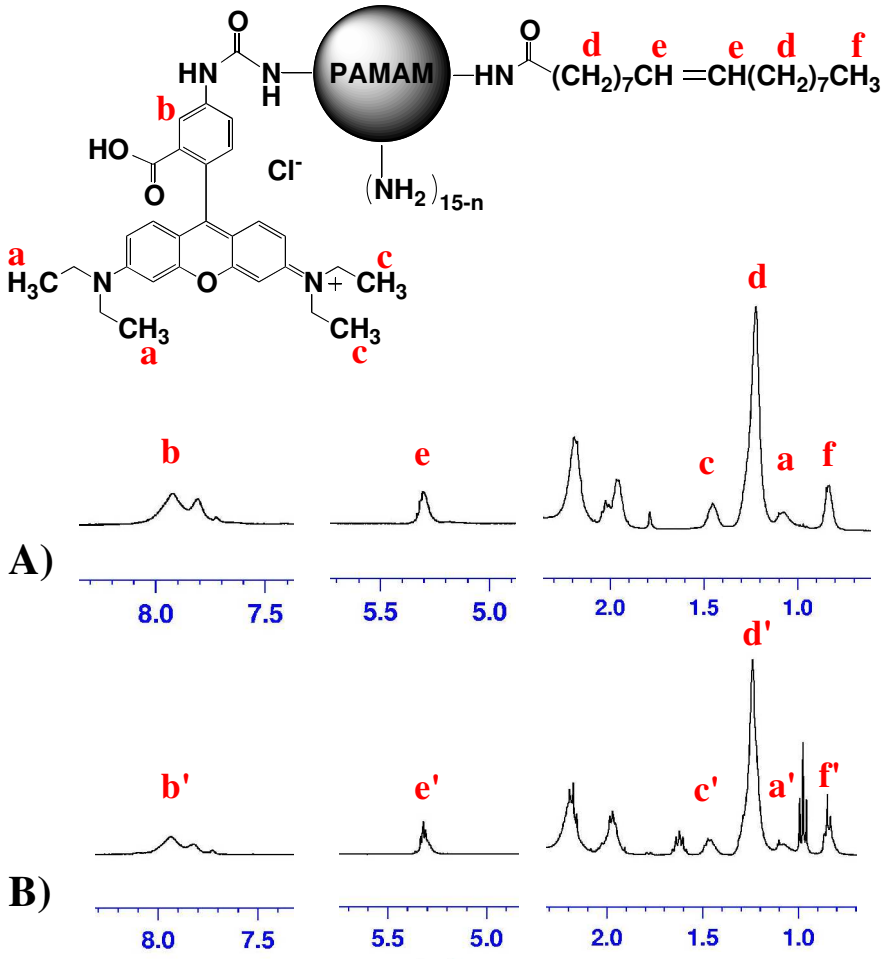

Figure S4. ^{1}H NMR spectra of G2-RITC-NH_2-OA for A) 1:5 reaction and B) 1:8 reaction

The large peak at 1.22 ppm (d and d') corresponds to the protons of the oleic acid backbone, and the peak at 0.89 ppm (f and f') is assigned to the methoxy end group of OA. The protons connected to the ethylene bond on oleic acid are observed at 5.30 ppm (e and e'). The methoxy groups in RITC are observed at 0.97 ppm (a and a') and 1.45 ppm (c and c'), and the proton peak at 7.92 ppm (b and b') corresponds to the protons on the benzene ring of RITC. The ratio of OA to RITC was calculated based on the integration values of the characteristic values. The measured ratios were ranging from A) 1:2 (the integration ratio of peak d or e to peak a or c) to 1:2.7 (the integration ratio of peak f to peak c) and B. 1:2.3 (the integration ratio of peak d' to peak c') to 1:3 (the integration ratio of peak e' to peak c').