

Supporting Information

Carbosilane Dendrimers Functionalized at the Periphery with Dansyl Fluorescence Tags and their Cellular Internalisation Studies.

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[Et₃Si(CH₂)₃NH(Dans)] (1)

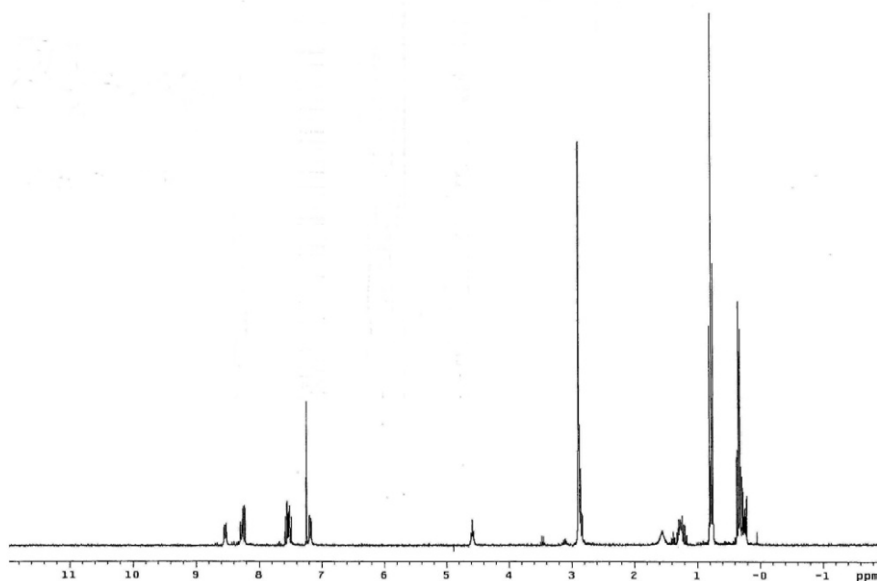


Figure S1. ¹H NMR spectrum of [Et₃Si(CH₂)₃NH(Dans)] (**1**) in CDCl₃.

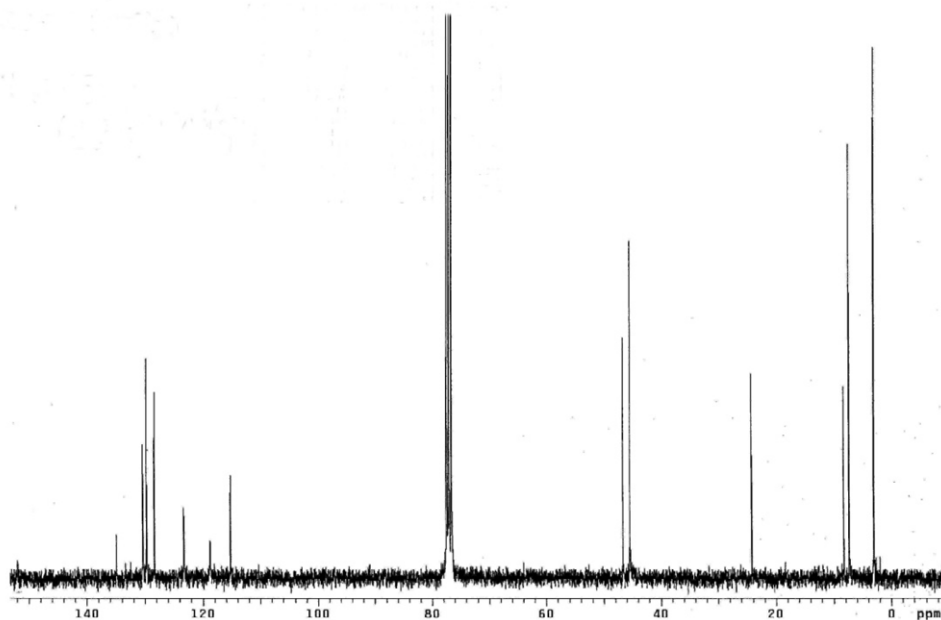


Figure S2. ¹³C NMR spectrum of [Et₃Si(CH₂)₃NH(Dans)] (**1**) in CDCl₃.

G₁-{[Si(CH₂)₃NH]Dansyl₄}
(2)

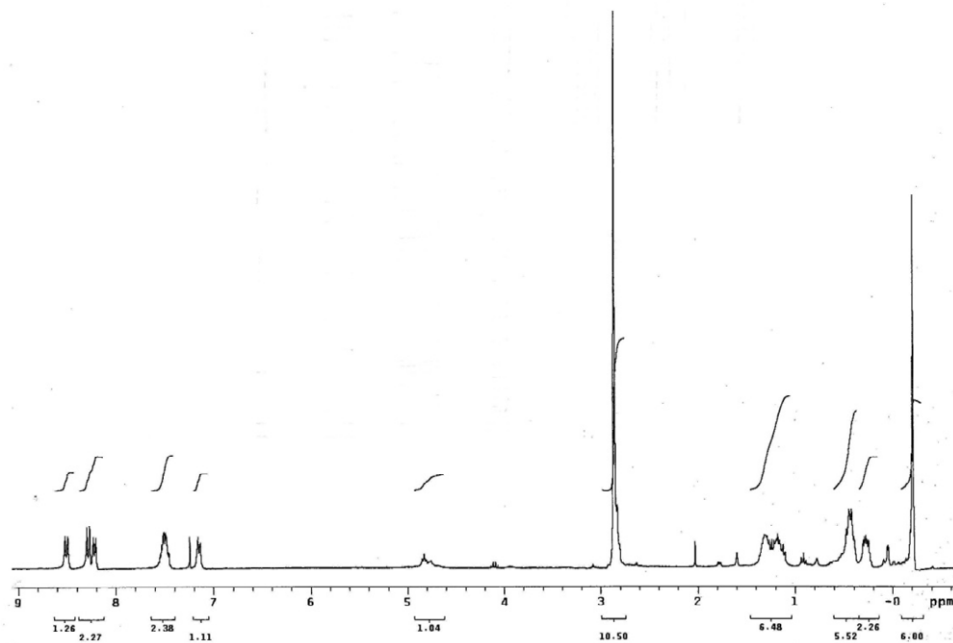


Figure S3. ¹H NMR spectrum of G₁-{[Si(CH₂)₃NH]Dansyl₄} (2) in CDCl₃.

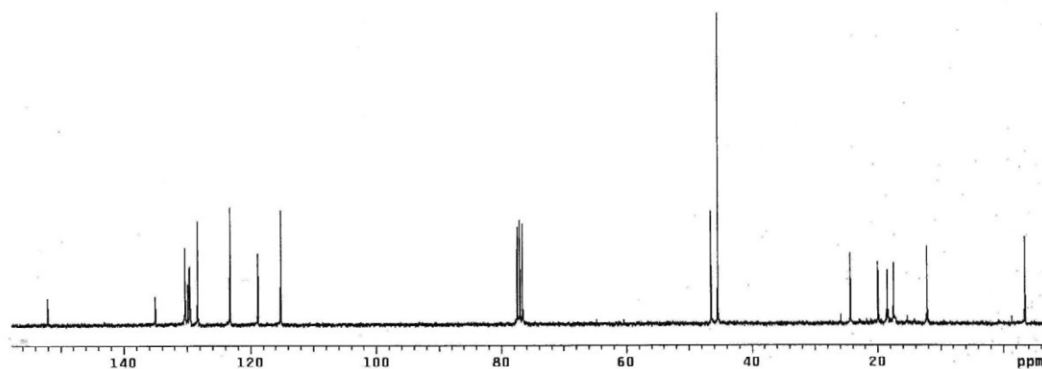


Figure S4. ¹³C NMR spectrum of G₁-{[Si(CH₂)₃NH]Dansyl₄} (2) in CDCl₃.

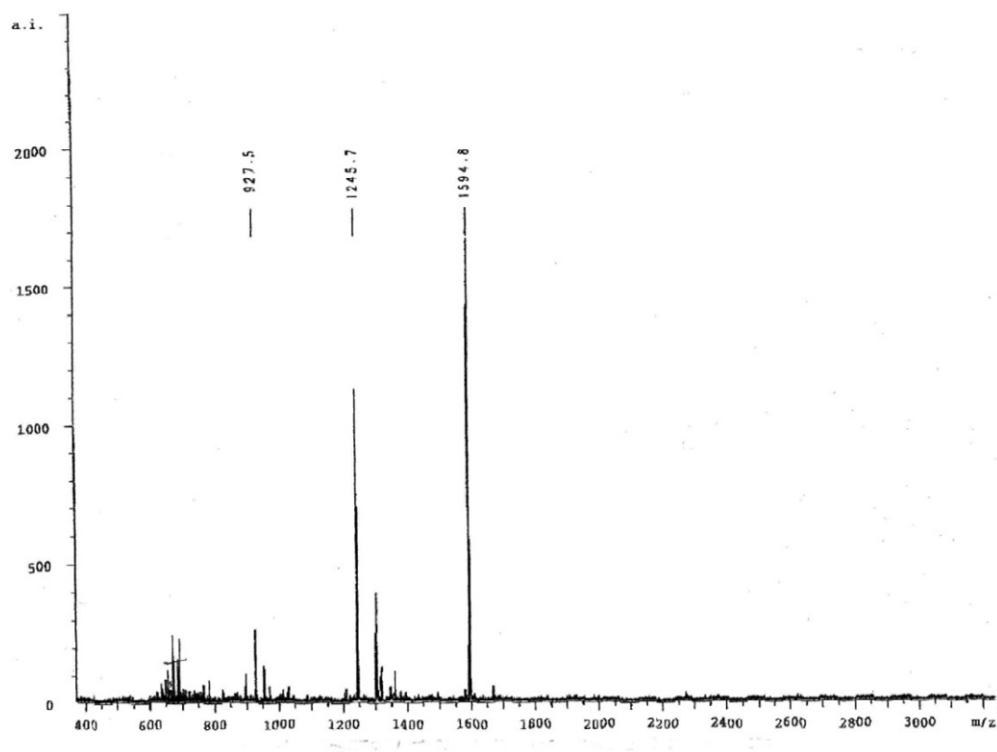


Figure S5. MALDI-TOF mass spectrometry of $G_1\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH})\text{Dansyl}]_4\}$ (**2**) in dithranol.

G₂-{[Si(CH₂)₃NH]Dansyl}₈} (3)

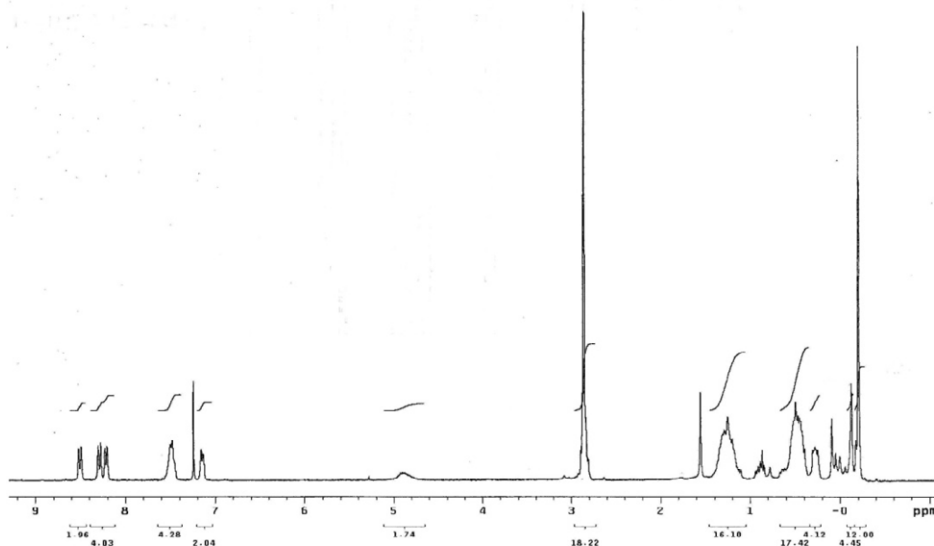


Figure S6. ¹H NMR spectrum of G₂-{[Si(CH₂)₃NH]Dansyl}₈ (3) in CDCl₃.

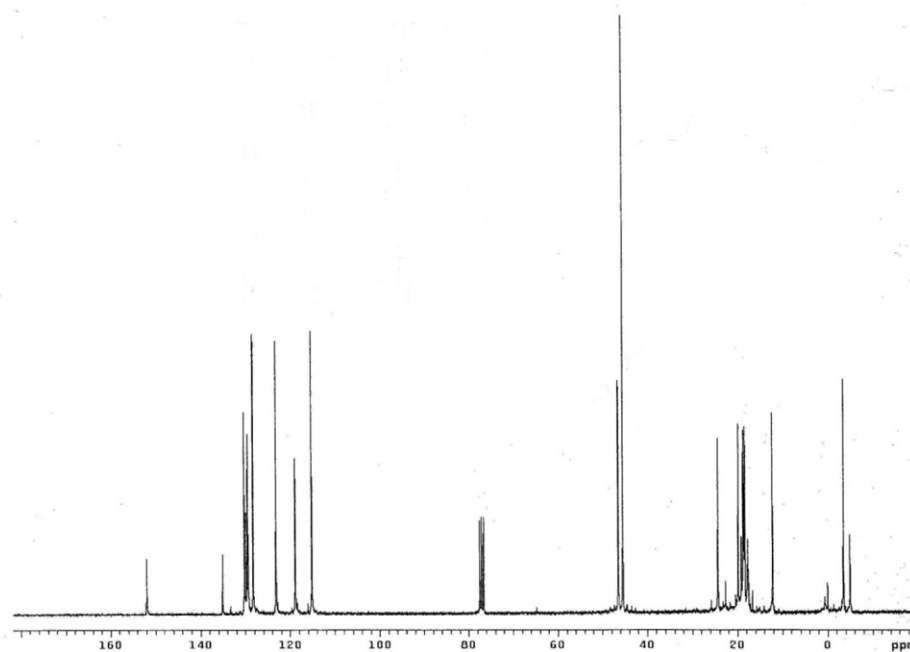


Figure S7. ¹³C NMR spectrum of G₂-{[Si(CH₂)₃NH]Dansyl}₈ (3) in CDCl₃.

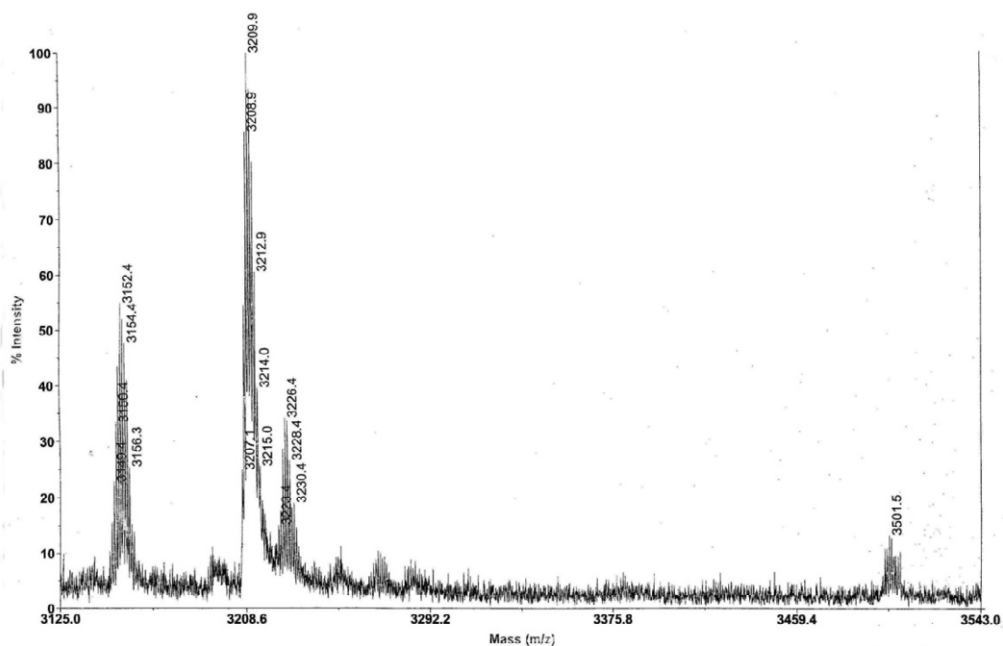


Figure S8. MALDI-TOF mass spectrometry of $G_2\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}]\text{Dansyl}\}_8$ (**3**) in dithranol.

G₃-{[Si(CH₂)₃NH]Dansyl]₁₆}
(4)

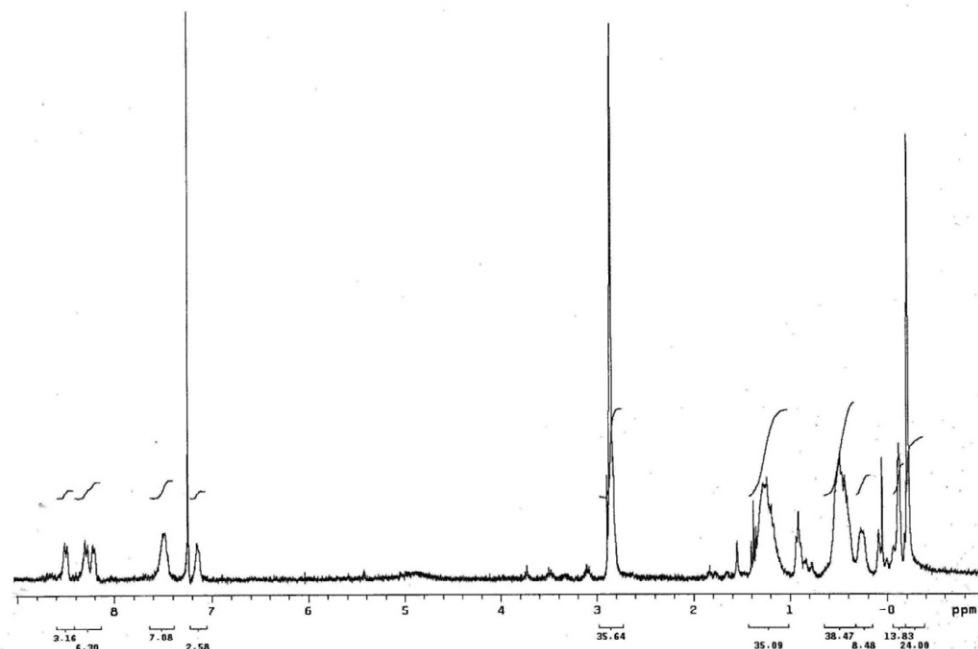


Figure S9. ¹H NMR spectrum of G₃-{[Si(CH₂)₃NH]Dansyl]₁₆} (**4**) in CDCl₃.

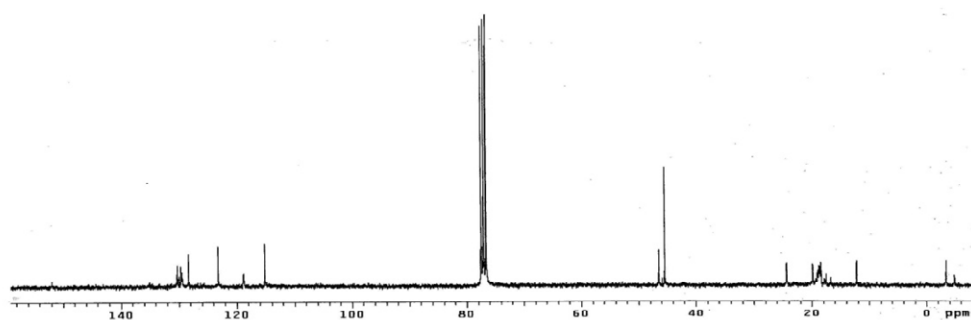


Figure S10. ¹³C NMR spectrum of G₃-{[Si(CH₂)₃NH]Dansyl]₁₆} (**4**) in CDCl₃.

G₂-{[Si(CH₂)₃NH₂]₅[Si(CH₂)₃NH]Dansyl]₃} (5)

x = % of dansyl groups per molecule
8-x = % of amino groups per molecule

$$\frac{[\% (NH_2)]}{[\% (Dans)]} = \frac{8-x}{x} \quad \frac{[\% (NH_2)]}{[\% (Dans)]} = \frac{\int_{\square} \left(\frac{Ha}{2}\right)}{\int_{\square} Hb} = \frac{1}{2}d$$

$$d = \frac{[\int_{\square} Ha]}{[\int_{\square} Hb]}$$

$$x = \frac{8}{\left[\left(\frac{1}{2}\right)d + 1\right]}$$

dansyl groups per molecule: x = 2,75
amino groups per molecule: y = 8-x = 5,25

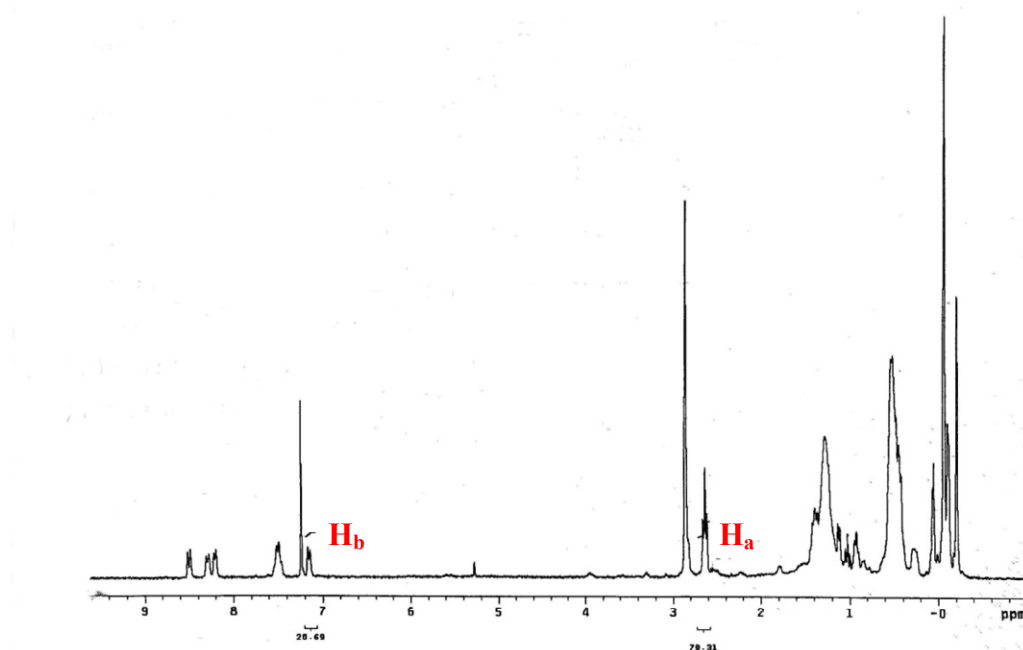


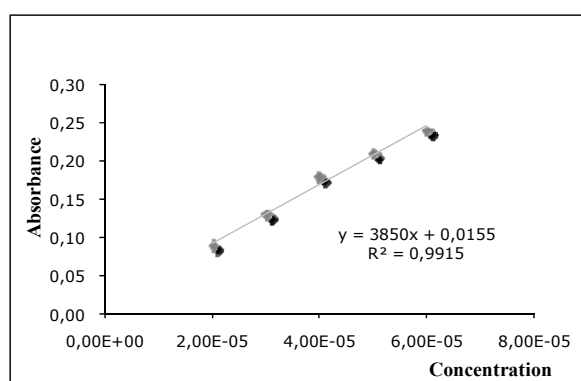
Figure S11. ¹H NMR spectrum of G₂-{[Si(CH₂)₃NH₂]₅[Si(CH₂)₃NH]Dansyl]₃} (5) in CDCl₃.

Calculation of number of branches containing amino or dansylated units via

UV-Vis spectra: molar extinction coefficient (ϵ)

Conc	Abs
2.00E-05	0.09
3.00E-05	0.13
4.00E-05	0.18
5.00E-05	0.21
6.00E-05	0.24

A) $[\text{Et}_3\text{Si}(\text{CH}_2)_3\text{NH}(\text{Dans})]$ (1)

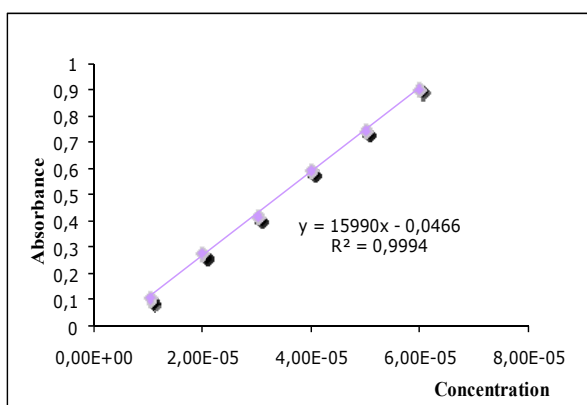


$$\epsilon = 3850$$

Figure S12. UV-VIS spectrum of $[\text{Et}_3\text{Si}(\text{CH}_2)_3\text{NH}(\text{Dans})]$ (1) in THF.

B) $G_1\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}(\text{Dansyl})]_4\}$ (2)

Conc	Abs
9.98E-06	0.11
1.99E-05	0.28
2.99E-05	0.42
3.99E-05	0.60
4.99E-05	0.75
5.99E-05	0.91



$$\epsilon = 15900$$

Quantification of chromophore groups : $15900 / 3850 = 4,12$

Theoretic = 4.0

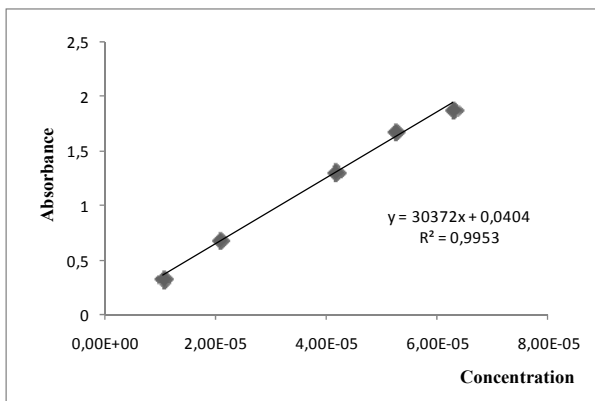
Experimental = 4.12

Figure S13. UV-VIS spectrum of $G_1\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}(\text{Dansyl})]_4\}$ (2) in THF.

C) G_2 -{[Si(CH₂)₃NH]Dansyl}₈} (3)

Conc.	Abs
1.05E-05	0.33
2.09E-05	0.69
4.18E-05	1.32
5.23E-05	1.69
6.28E-05	1.89

$$\epsilon = 30372$$



Quantification of chromophore groups: $30372 / 3850 = 7.88$

Theoretic = 8.0

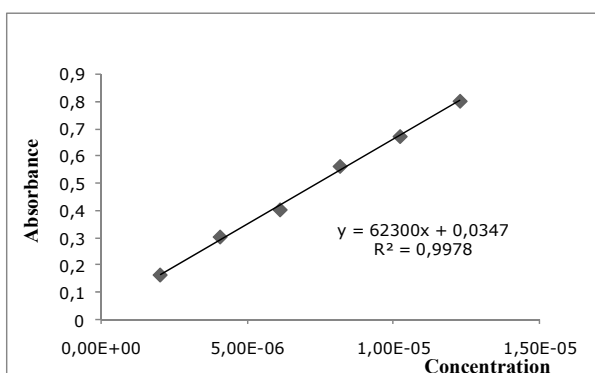
Experimental = 7.88

Figure S14. UV-VIS spectrum of G_2 -{[Si(CH₂)₃NH]Dansyl}₈} (3) in THF.

D) G_3 -{[Si(CH₂)₃NH]Dansyl}₁₆} (4)

Conc.	Abs.
2.05E-06	0.16
4.10E-06	0.30
6.15E-06	0.40
8.20E-06	0.56
1.03E-05	0.67
1.23E-05	0.80

$$\epsilon = 62300$$



Quantification of chromophore groups: $62300 / 3850 = 16.1$

Theoretic = 16.0

Experimental = 16.1

Figure S15. UV-VIS spectrum of G_3 -{[Si(CH₂)₃NH]Dansyl}₁₆} (4) in THF.

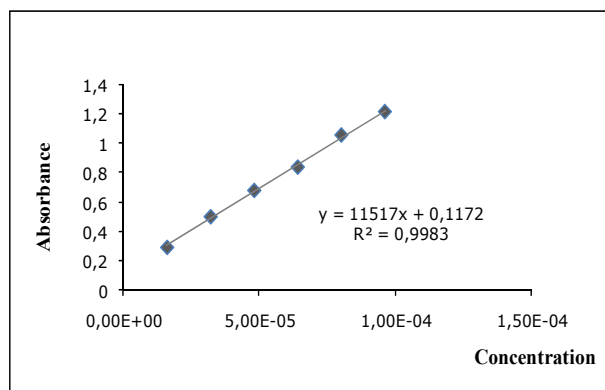
E) $G_2\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}_2]_5[\text{Si}(\text{CH}_2)_3\text{NH})\text{Dansyl}\}_3$ (5)

Formula (calculated by ^1H RMN): $2\text{G}(\text{NH}_2)_{5.2}(\text{DNS})_{2.8}$

Estimated Mw: 2277.03 g/mol

Conc.	Abs.
1,60E-05	0,29
3,21E-05	0,5
4,82E-05	0,68
6,43E-05	0,84
8,04E-05	1,06
9,65E-05	1,22

$$\epsilon = 11517$$



Quantification of chromophore groups: $11517 / 3850 = 2.99$

Theoretic = 3.0

Experimental = 2.99

Figure S16. UV-VIS spectrum of $G_2\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}_2]_5[\text{Si}(\text{CH}_2)_3\text{NH})\text{Dansyl}\}_3$ (5) in THF.

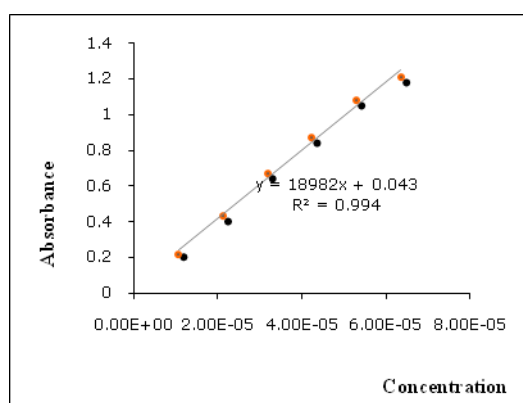
F) $G_2\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}_2]_3[\text{Si}(\text{CH}_2)_3\text{NH})\text{Dansyl}\}_5$ (6)

Formula (calculated by ^1H RMN): $2\text{G}(\text{NH}_2)_{2.6}(\text{DNS})_{5.4}$

Estimated Mw: 2911.47 g/mol

conc	Abs
1.06E-05	0.23
2.12E-05	0.43
3.18E-05	0.67
4.24E-05	0.87
5.30E-05	1.08
6.37E-05	1.21

$$\epsilon = 18982$$



Quantification of chromophore groups: $18982 / 3850 = 4.93$

Theoretic = 5.0

Experimental = 4.93

Figure S17. UV-VIS spectrum of $G_2\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}_2]_3[\text{Si}(\text{CH}_2)_3\text{NH})\text{Dansyl}\}_5$ (6) in THF.

GPC traces of dendrimers 2-6

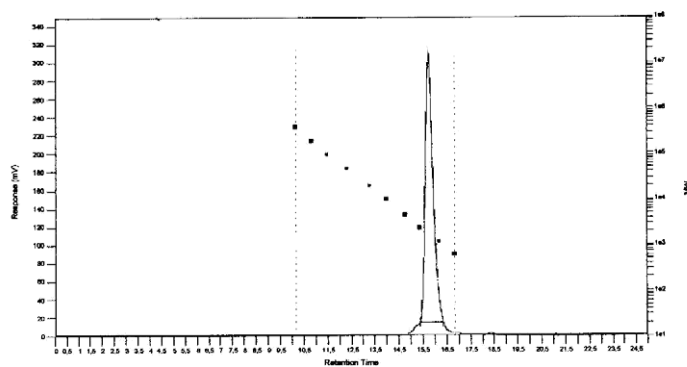


Fig S18. GPC trace of G₁-{[Si(CH₂)₃NH)Dansyl]₄} (2).

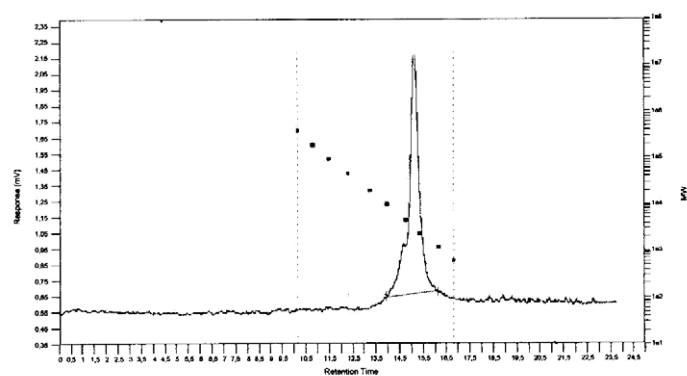


Fig S19. GPC trace of G₂-{[Si(CH₂)₃NH)Dansyl]₈} (3).

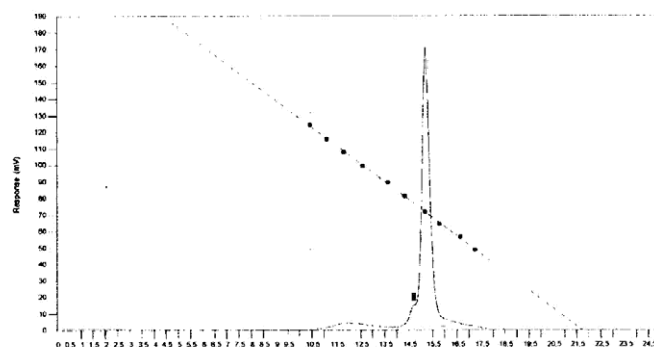


Fig S20. GPC trace of G₃-{[Si(CH₂)₃NH)Dansyl]₁₆} (4).

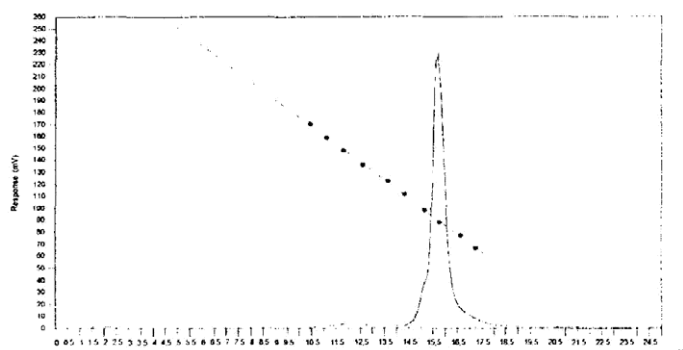


Fig S21. GPC trace of $G_2\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}_2]_5[\text{Si}(\text{CH}_2)_3\text{NH})\text{Dansyl}]_3\}$ (**5**).

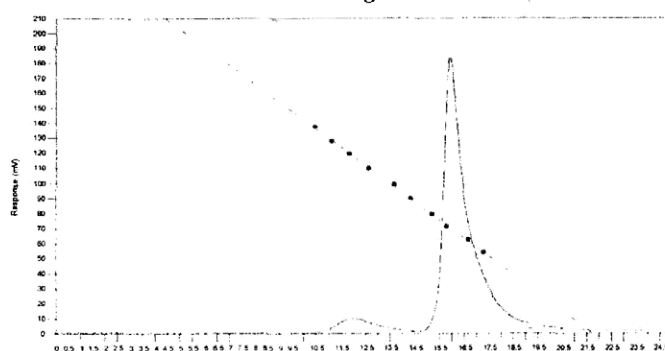


Fig S22. GPC trace of $G_2\text{-}\{[\text{Si}(\text{CH}_2)_3\text{NH}_2]_3[\text{Si}(\text{CH}_2)_3\text{NH})\text{Dansyl}]_5\}$ (**6**).

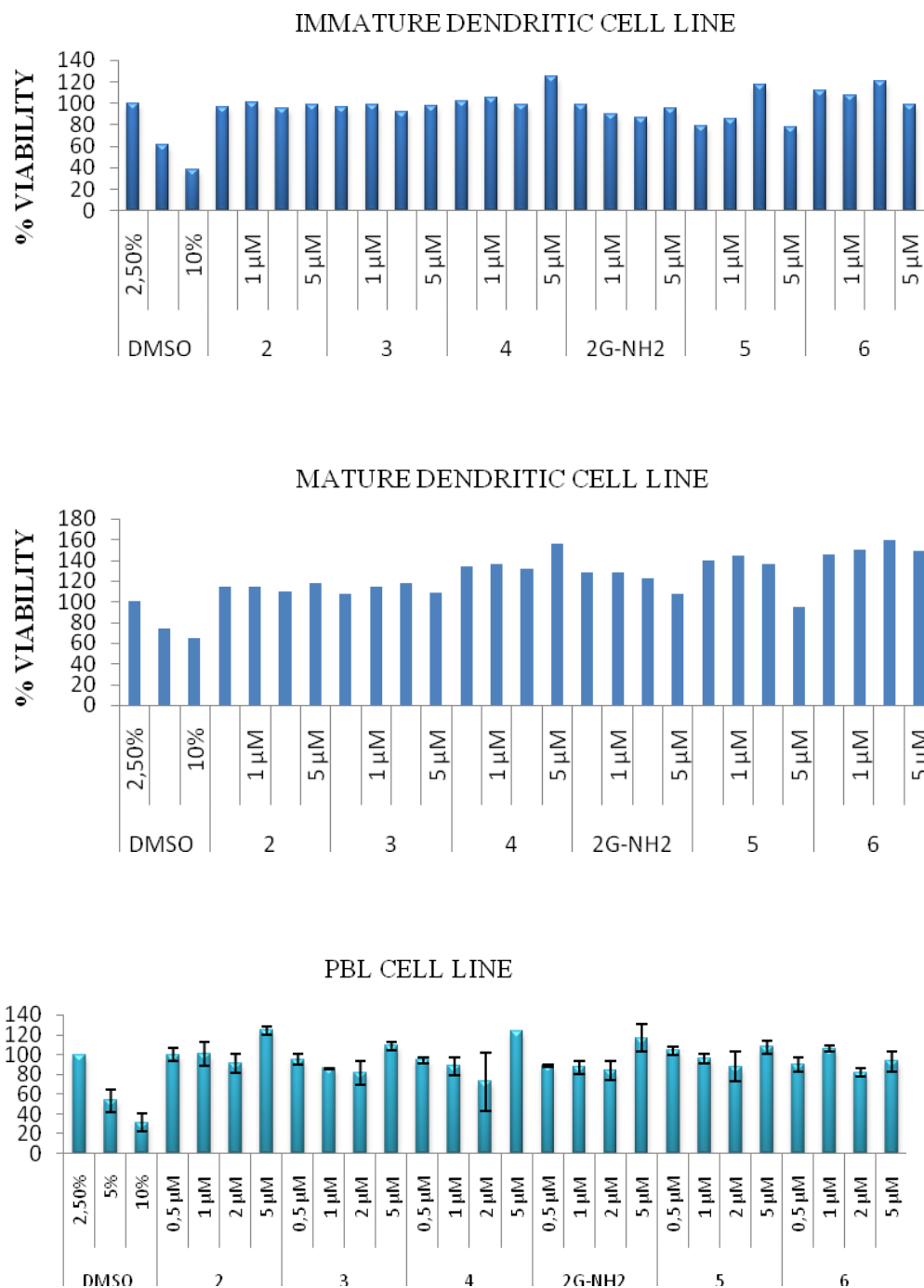


Figure S23. Toxicity assays of dendrimers **2-6** on different cell lines performed by MTT test. Dendrimer 2G-NH2 correspond to the starting material G₂-[Si(CH₂)₃NH₂]₈.