

SUPPORTING INFORMATION

"SYNTHESIS, CARACTHERIZATION AND ANTIBACTERIAL BEHAVIOR OF WATER-SOLUBLE CARBOSILANE DENDRONS CONTAINING FERROCENE AT THE FOCAL POINT"

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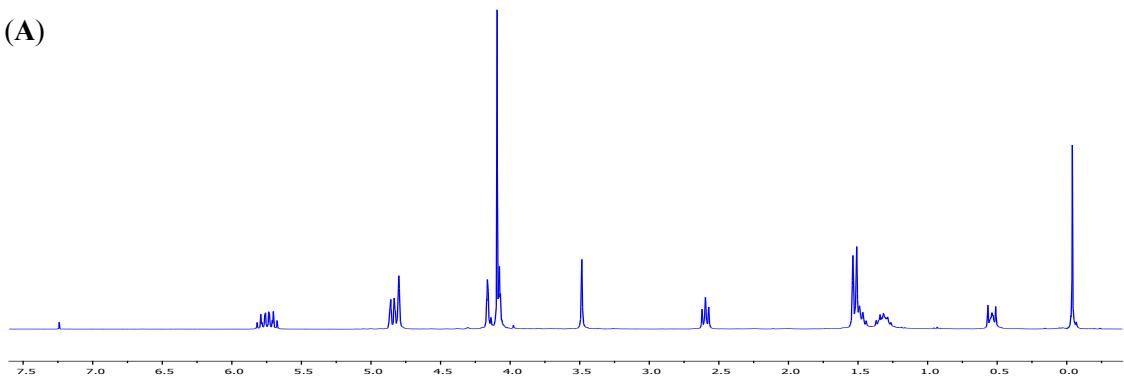
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$\text{FcCH}_2\text{NH}(\text{CH}_2)_4[\text{G}_1(\text{Allyl})_2]$ (1)

(A)



(B)

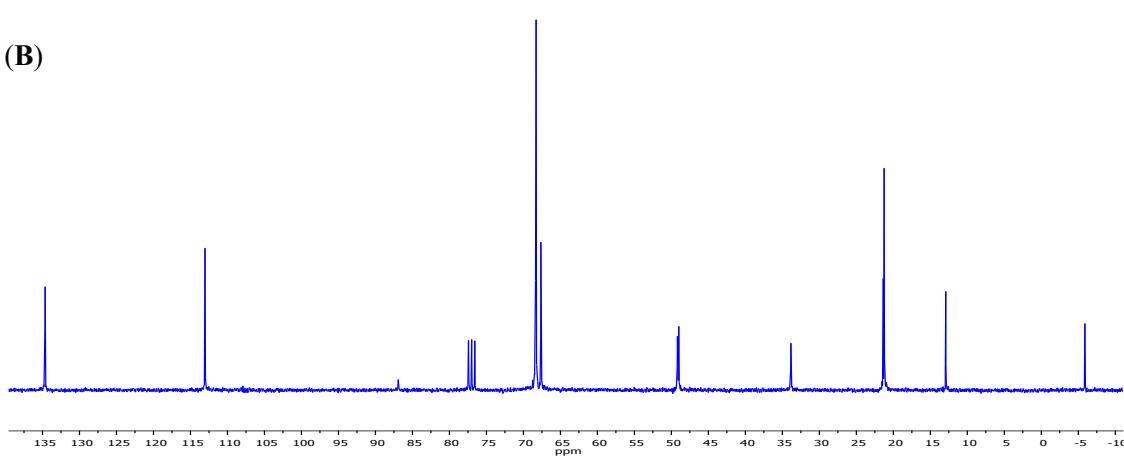


Figure 1S. (A) ¹H and (B) ¹³C-NMR spectra of $\text{FcCH}_2\text{NH}(\text{CH}_2)_4[\text{G}_1(\text{Allyl})_2]$ (1) in CDCl_3 .

FeCH₂NH(CH₂)₄[G₂(Allyl)₄] (2)

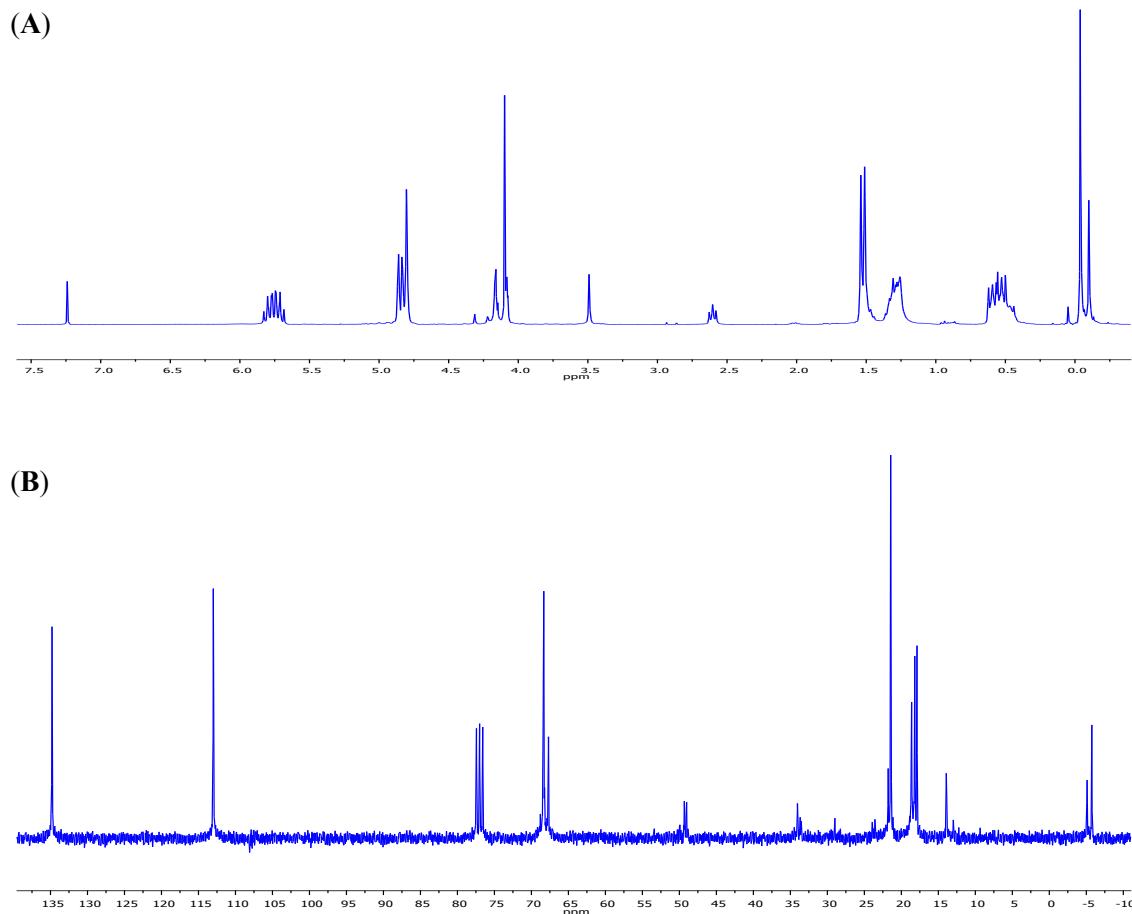


Figure 2S. (A) ¹H and (B) ¹³C-NMR spectra of FeCH₂NH(CH₂)₄[G₂(Allyl)₄] (2) in CDCl₃.

FeCH₂NH(CH₂)₄[G₃(Allyl)₈] (3)

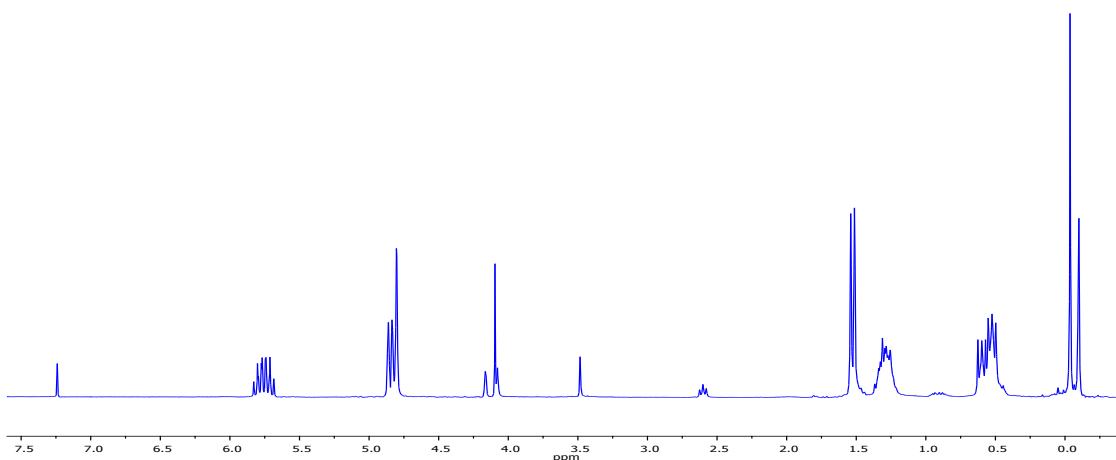
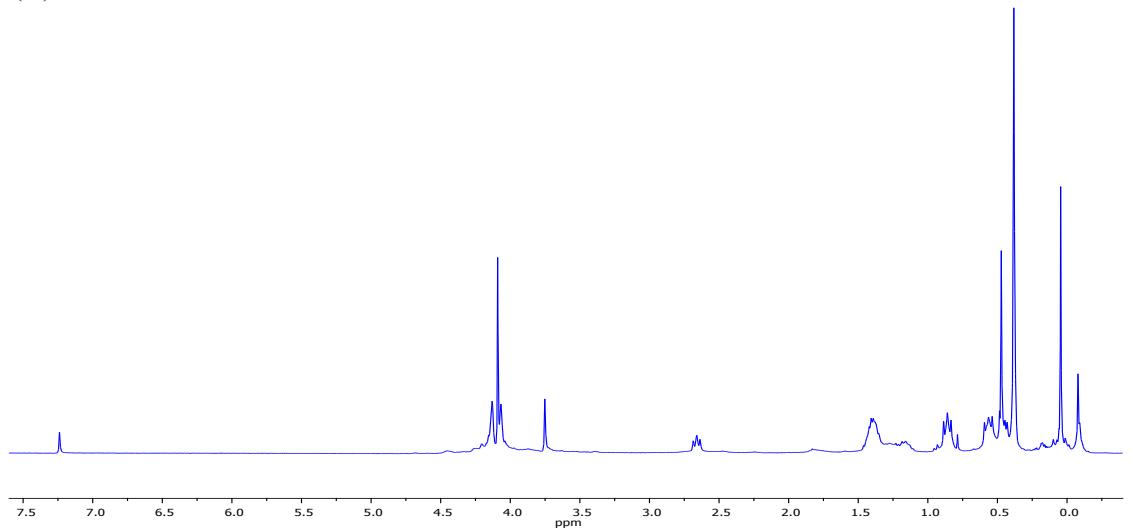


Figure 3S. ¹H-NMR spectrum of FeCH₂NH(CH₂)₄ [G₃(Allyl)₈] (3) in CDCl₃.

FeCH₂NH(CH₂)₄[G₁(SiMe₂Cl)₂] (4)

(A)



(B)

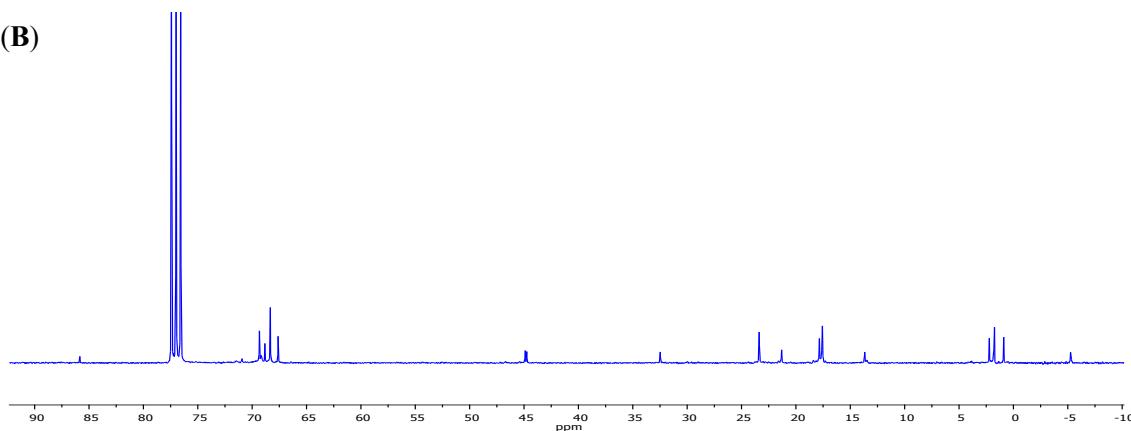


Figure 4S. (A) ¹H and (B) ¹³C-NMR spectra of FeCH₂NH(CH₂)₄[G₁(SiMe₂Cl)₂] (4) in CDCl₃.

FeCH₂NH(CH₂)₄[G₂(SiMe₂Cl)₄] (5)

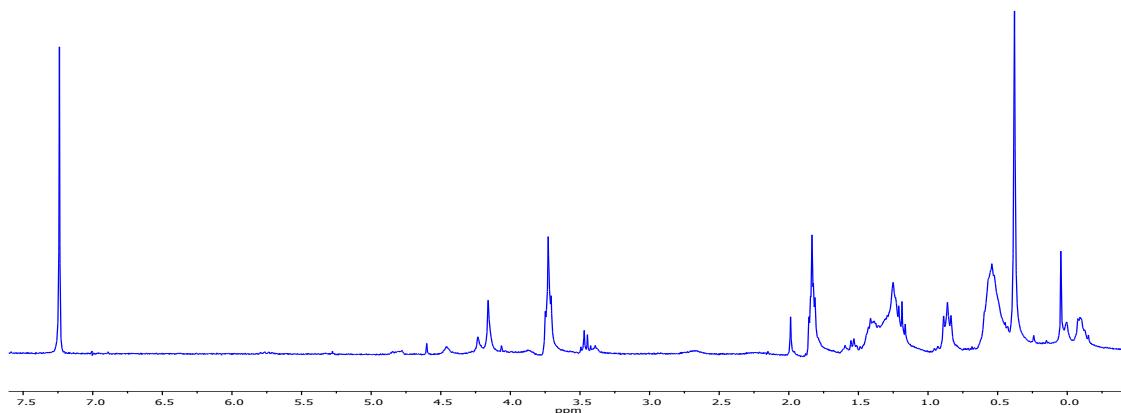
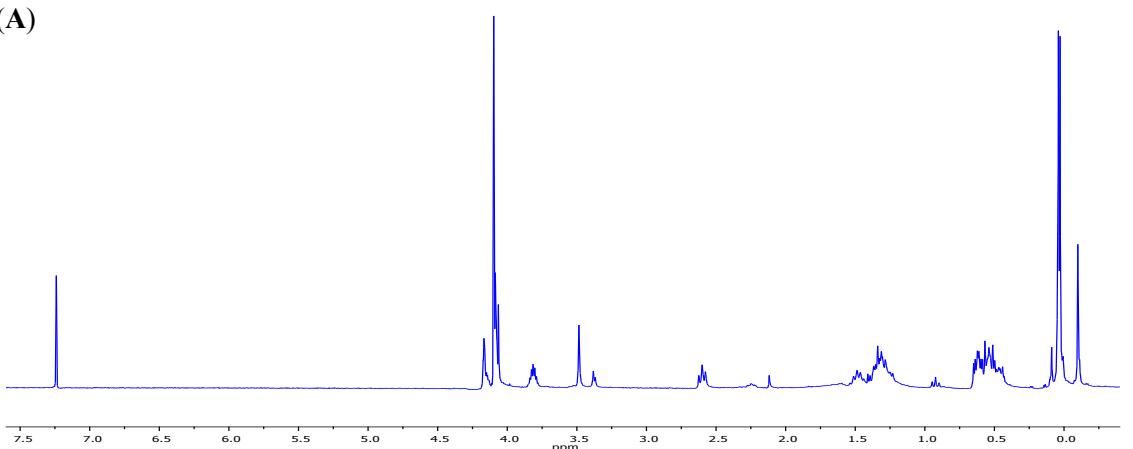


Figure 5S. ¹H-NMR spectrum of FeCH₂NH(CH₂)₄[G₂(SiMe₂Cl)₄] (5) in CDCl₃.

FcCH₂NH(CH₂)₄[G₁(SiMe₂H)₂] (7)

(A)



(B)

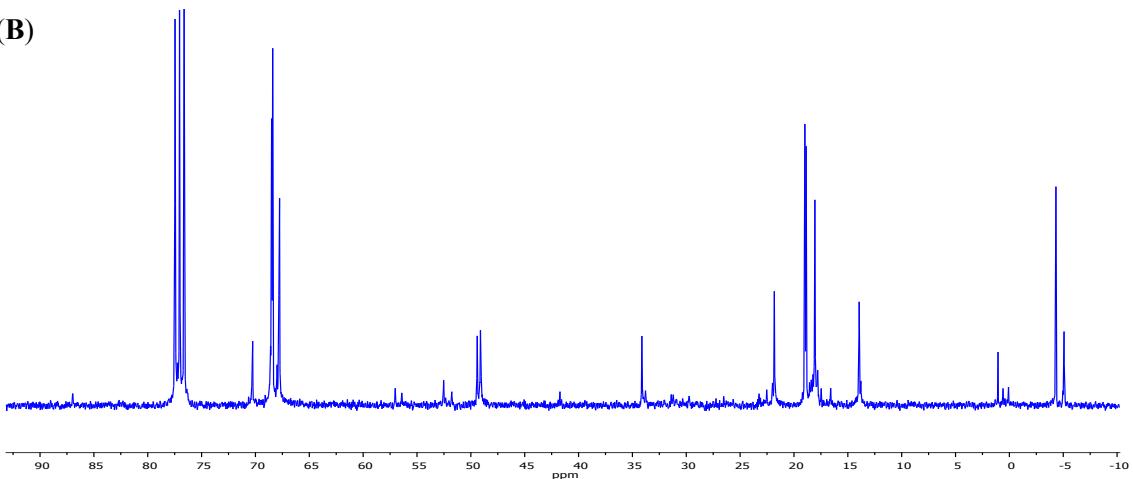


Figure 6S. (A) ¹H and (B) ¹³C-NMR spectra of FcCH₂NH(CH₂)₄[G₁(SiMe₂H)₂] (7) in CDCl₃.

FcCH₂NH(CH₂)₄[G₂(SiMe₂H)₄] (8)

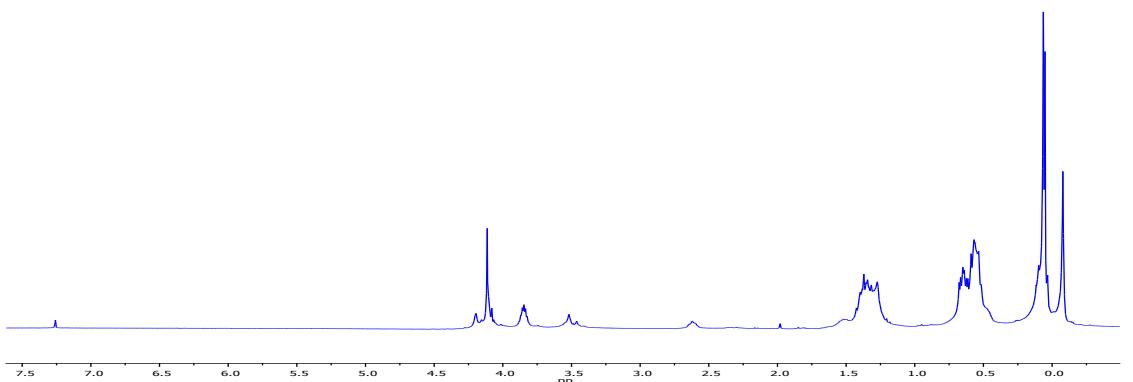
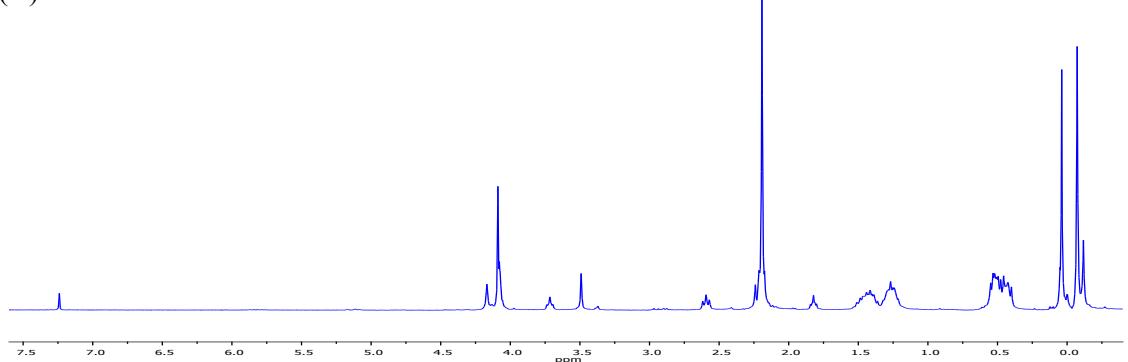


Figure 7S. ¹H-NMR spectrum of FcCH₂NH(CH₂)₄[G₂(SiMe₂H)₄] (8) in CDCl₃.

FeCH₂NH(CH₂)₄[G₁(SiMe₂(CH₂)₃NMe₂)₂] (10)

(A)



(B)

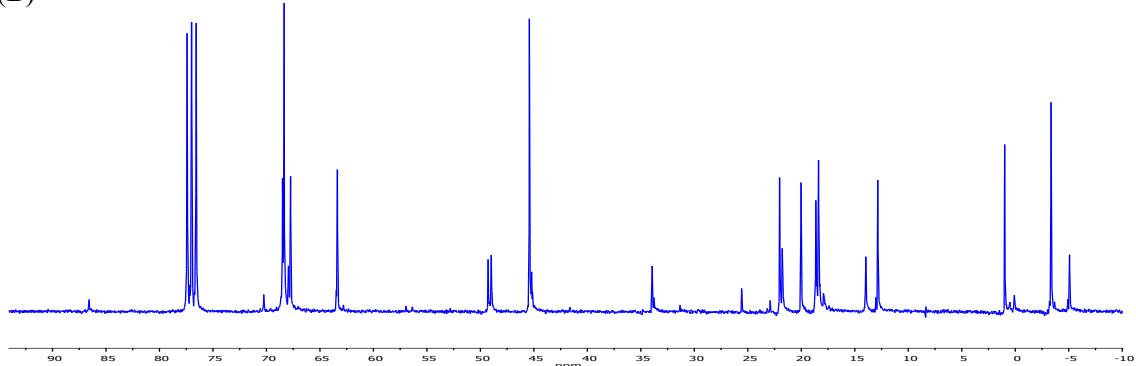
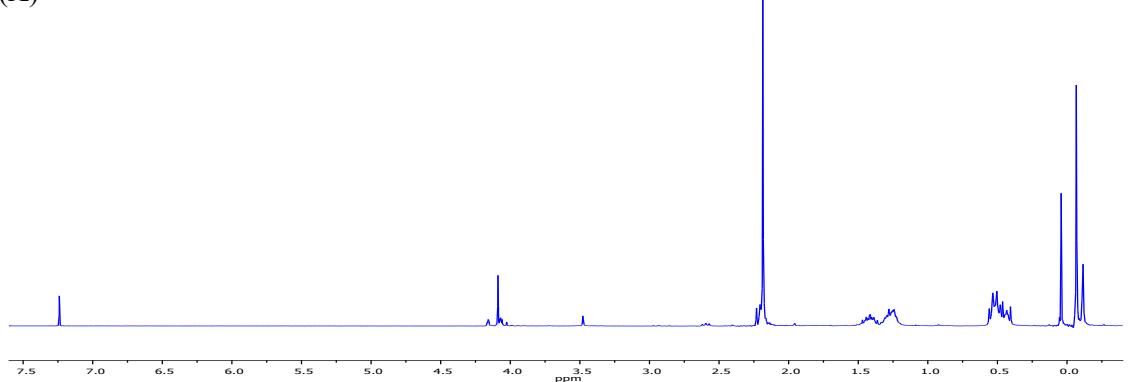


Figure 8S. (A) ¹H and (B) ¹³C-NMR spectra of FeCH₂NH(CH₂)₄[G₁(SiMe₂(CH₂)₃NMe₂)₂] (10) in CDCl₃.

FeCH₂NH(CH₂)₄[G₂(SiMe₂(CH₂)₃NMe₂)₄] (11)

(A)



(B)

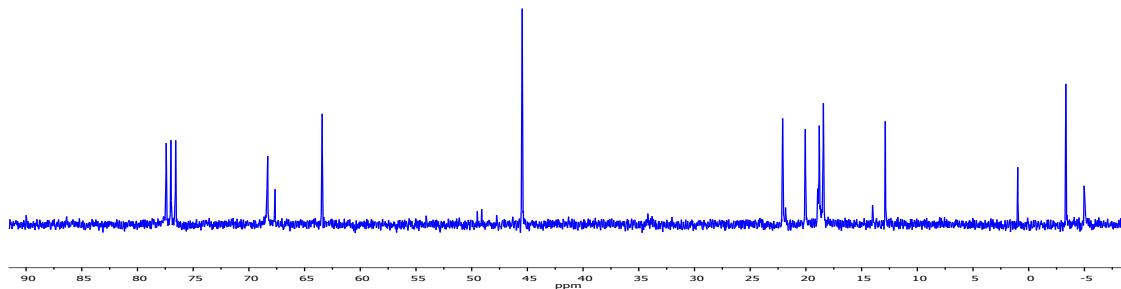
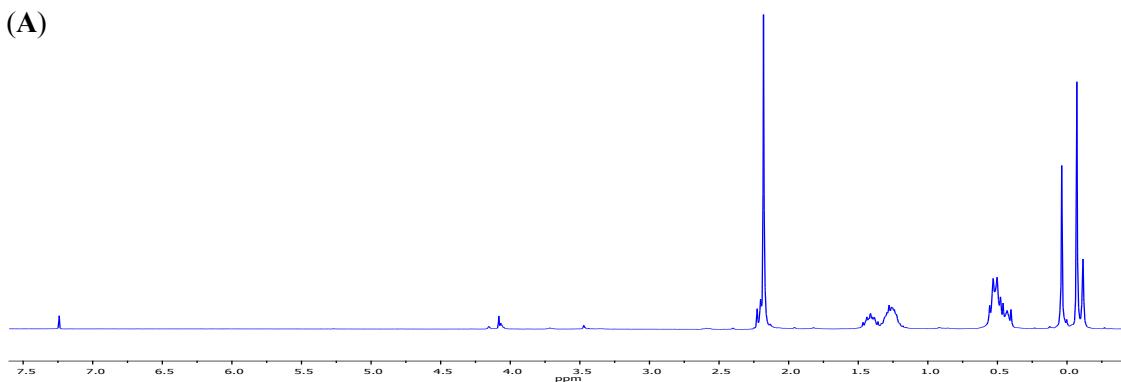


Figure 9S. (A) ¹H and (B) ¹³C-NMR spectra of $\text{FcCH}_2\text{NH}(\text{CH}_2)_4[\text{G}_2(\text{SiMe}_2(\text{CH}_2)_3\text{NMe}_2)_4]$ (**11**) in CDCl_3 .

FcCH₂NH(CH₂)₄[G₃(SiMe₂(CH₂)₃NMe₂)₈] (12)

(A)



(B)

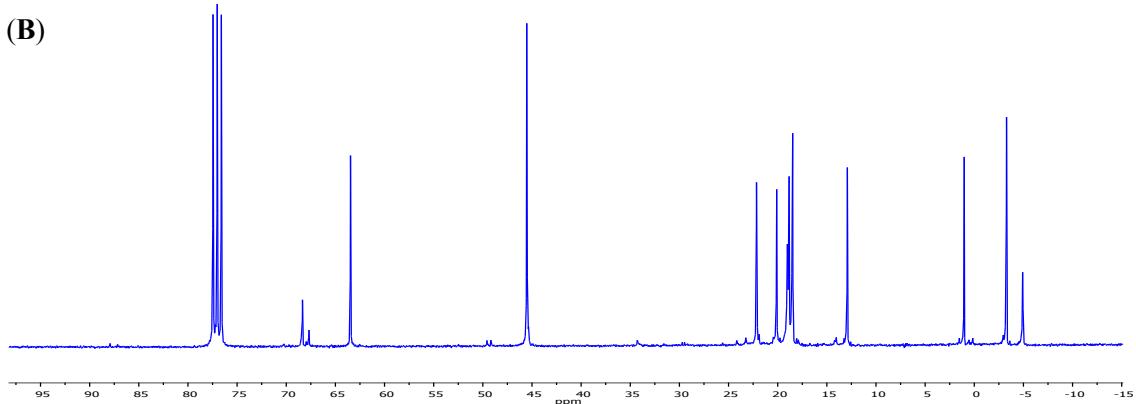


Figure 10S. (A) ¹H and (B) ¹³C-NMR spectra of $\text{FcCH}_2\text{NH}(\text{CH}_2)_4[\text{G}_3(\text{SiMe}_2(\text{CH}_2)_3\text{NMe}_2)_8]$ (**12**) in CDCl_3 .

FcCH₂NH₂Cl(CH₂)₄[G₁(SiMe₂(CH₂)₃NHMe₂Cl)₂] (13)

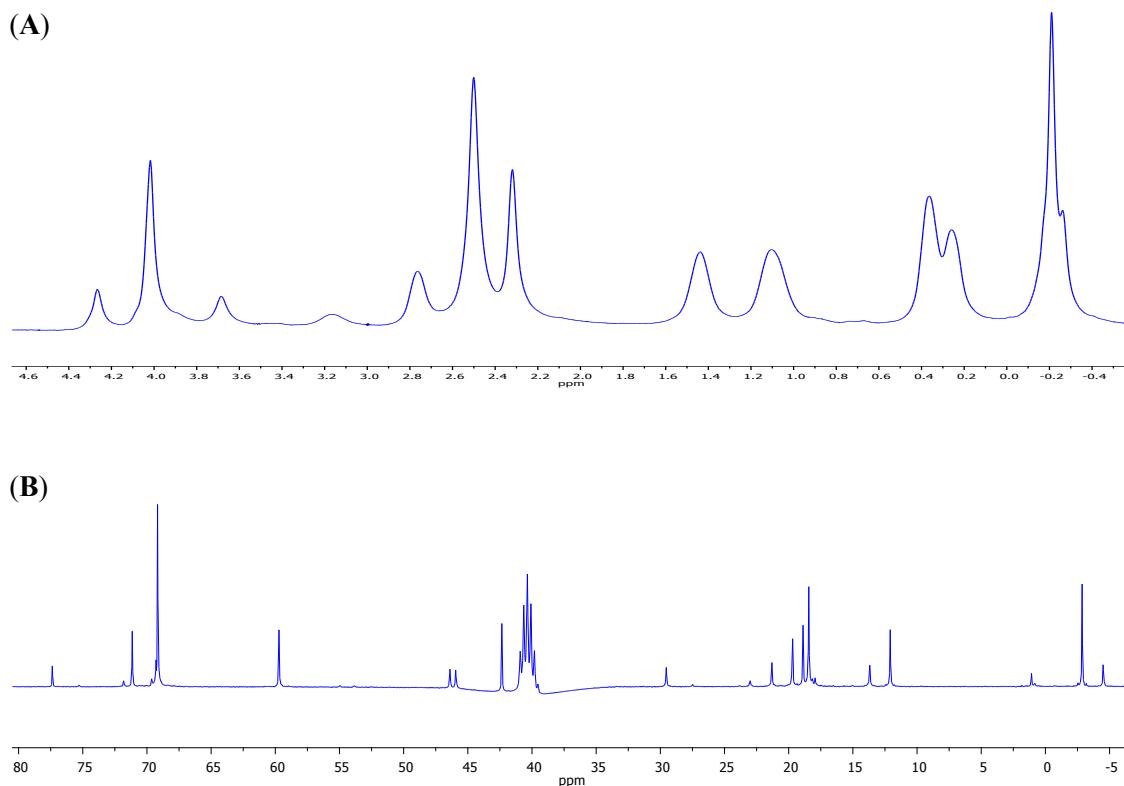


Figure 11S. (A) ¹H and (B) ¹³C-NMR spectra of FcCH₂NH₂Cl(CH₂)₄[G₁(SiMe₂(CH₂)₃NHMe₂Cl)₂] (13) in DMSO-*d*₆.

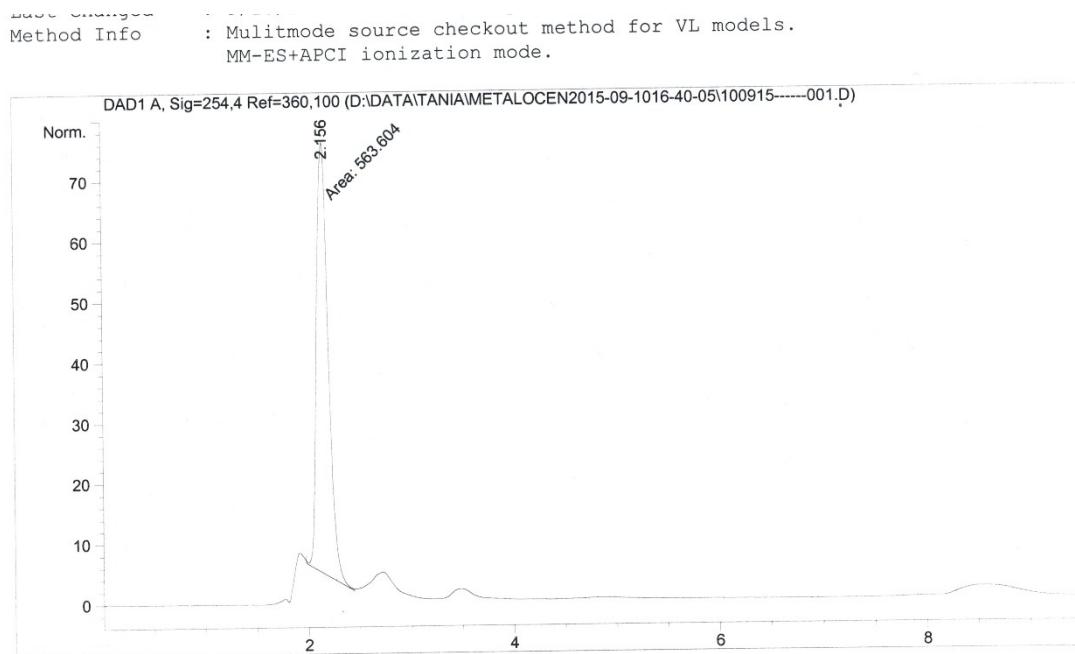


Figure 12S. HPLC (70% MeOH/30%TFA) chromatogram of FcCH₂NH₂Cl(CH₂)₄[G₁(SiMe₂(CH₂)₃NHMe₂Cl)₂] (13).

FcCH₂NH₂Cl(CH₂)₄[G₂(SiMe₂(CH₂)₃NHMe₂Cl)₄] (14)

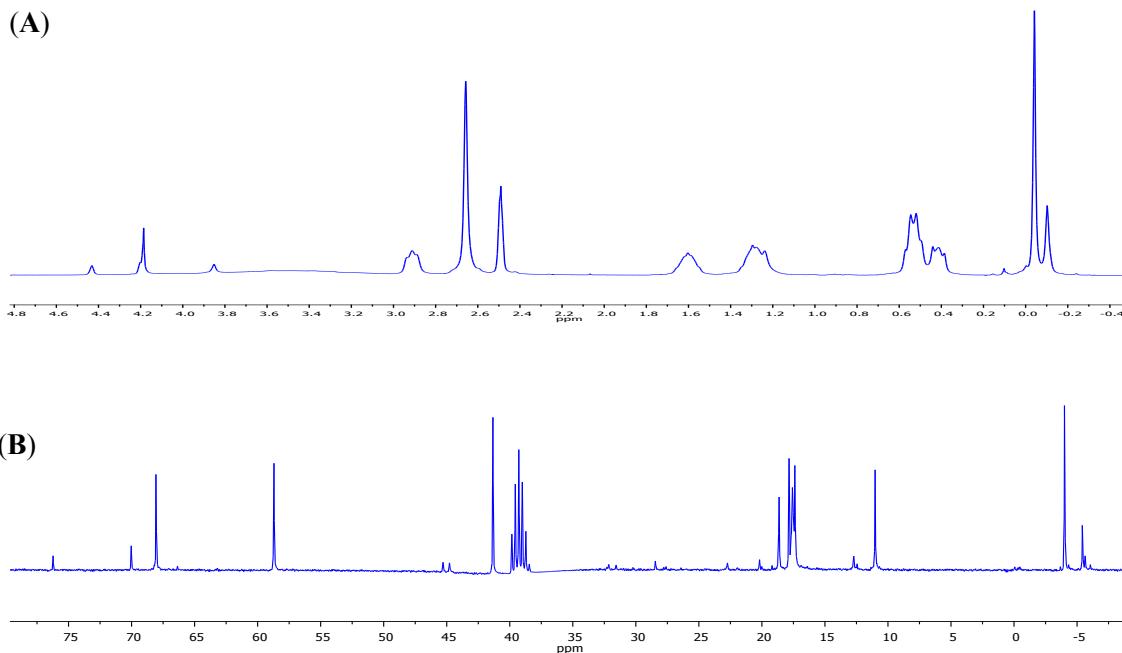


Figure 13S. (A) ¹H and **(B)** ¹³C-NMR spectra of FcCH₂NH₂Cl(CH₂)₄[G₂(SiMe₂(CH₂)₃NHMe₂Cl)₄] (**14**) in DMSO-d₆.

Method Info : Multimode source checkout method for VL models.
MM-ES+APCI ionization mode.

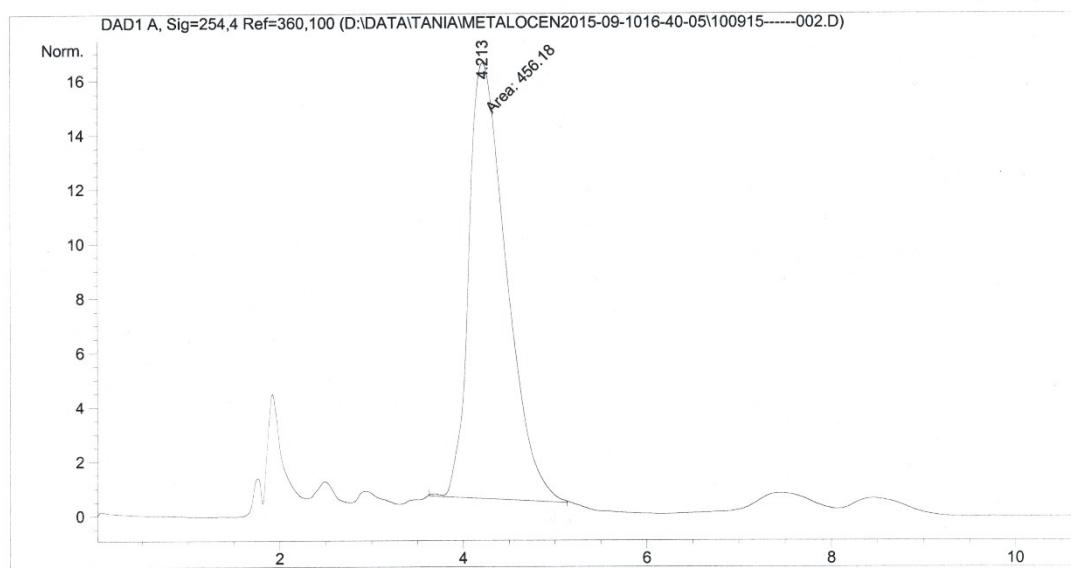


Figure 14S. HPLC (70% MeOH/30%TFA) chromatogram of FcCH₂NH₂Cl(CH₂)₄[G₂(SiMe₂(CH₂)₃NHMe₂Cl)₄] (**14**)

FcCH₂NH₂Cl(CH₂)₄[G₃(SiMe₂(CH₂)₃NHMe₂Cl)₈] (15)

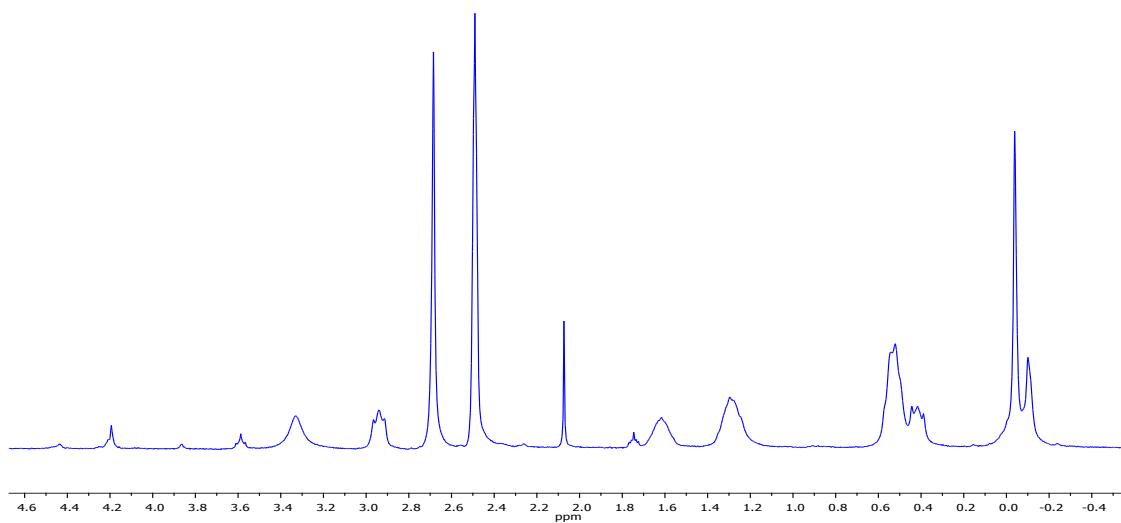


Figure 15S. ¹H-NMR spectrum of FcCH₂NH₂Cl(CH₂)₄[G₃(SiMe₂(CH₂)₃NHMe₂Cl)₈] (15) in DMSO-*d*₆.

(ClNH₃)(CH₂)₄[G₁(SiMe₂(CH₂)₃NHMe₂Cl)₂] (16)

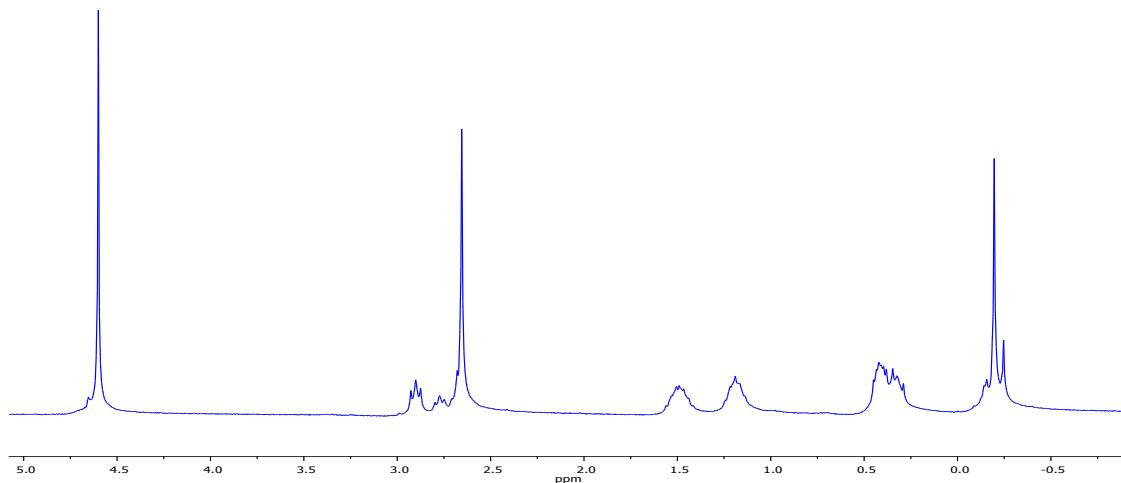


Figure 16S. ¹H-NMR spectrum of (ClNH₃)(CH₂)₄[G₁(SiMe₂(CH₂)₃NHMe₂Cl)₂] (16) in D₂O.

Synthesis of $\text{FcCH}_2\text{NH}_2(\text{Cl})(\text{CH}_2)_4\text{Si}(\text{Me}_2)(\text{CH}_2)\text{NMe}_2\text{HCl}$ (F)

To prepare F, reaction sequences following those of dendritic wedge 16 and allyl compounds (1, 2 and 3) were combined.

Compound A: starting from (2.2 mmol) of 4-bromo-1-butene and 0.38 mL of chlorodimethylsilane and LiAlH₄ (1.30 mL, 2.61 mmol) to obtain A (1.6 mmol, 72 %).

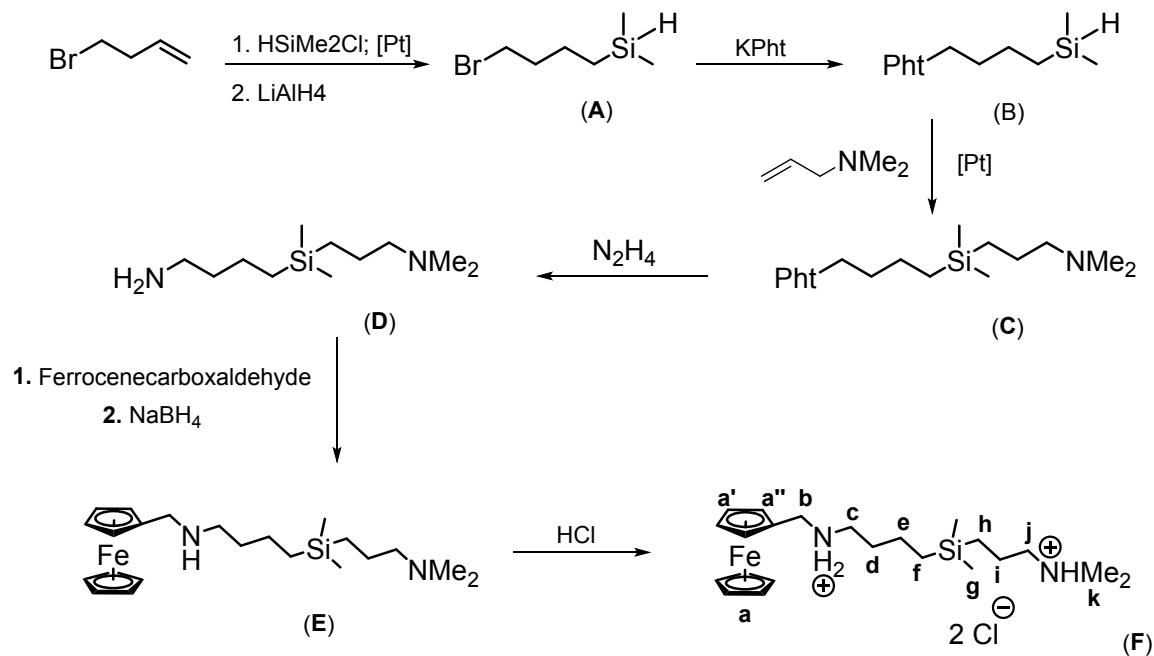
Compound B: starting from a solution of A in DMF (1.6 mmol) and KPh_t (2.2 mmol, 0.42 g) and 10% NaI. To obtain B (1.5 mmol, 93%).

Compound C: starting from B (1.5 mmol) and excess N,N-dimethylallylamine (2.0 mmol) to obtain C (1.3 mmol, 86%).

Compound D: starting from C (1.3 mmol) and N₂H₄ (0.10 mL, 3.32 mmol) to obtain D (0.9 mmol, 70%)

Compound E: starting from D (0.9 mmol) and ferrocenecarboxaldehyde (0.19 g, 0.9 mmol) to obtain E (0.7 mmol, 77%).

Compound F: starting from E (0.7 mmol) and HCl (2M in Et₂O, 1.2 mL, 2.35 mmol) to obtain F (0.7 mmol, 100%). Anal. Calcd for C₂₂H₃₉Cl₂FeN₂Si: C, 54.33; H, 8.08; N, 5.76; Exp: C, 54.63; H, 8.10; N, 5.93.



Scheme 1S. Synthesis of $\text{FcCH}_2\text{NH}_2\text{Cl}(\text{CH}_2)_4\text{Si}(\text{Me}_2)(\text{CH}_2)\text{NMe}_2\text{Cl}$ (F)

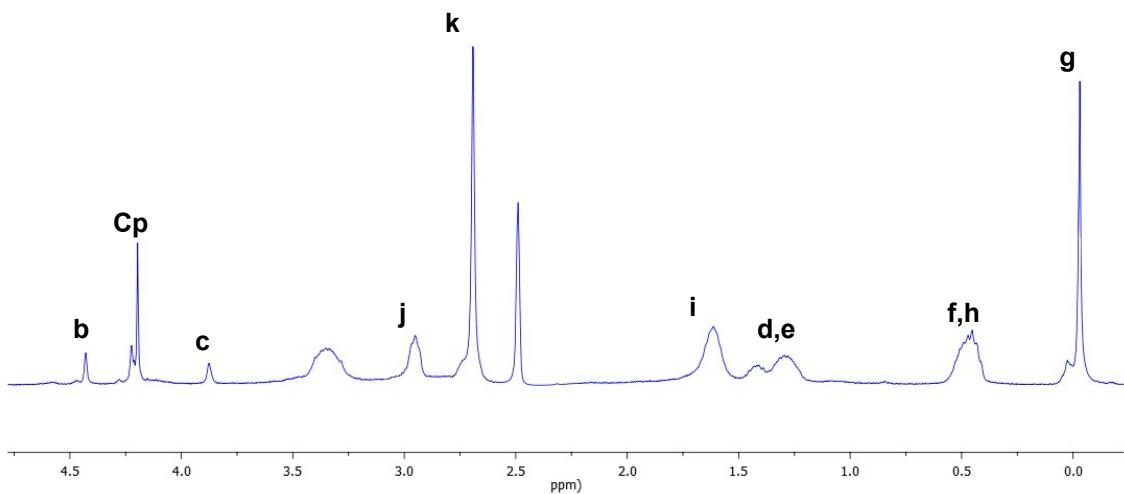


Figure 15S. ¹H-NMR spectrum of $\text{FcCH}_2\text{NH}_2\text{Cl}(\text{CH}_2)_4\text{SiMe}_2(\text{CH}_2)_3\text{NHMe}_2\text{Cl}$ (**F**) in $\text{DMSO}-d_6$.