

Supporting Information

A Monomolecularly Imprinted Dendrimer (MID) Capable of Selective Binding with a Tris(2-aminoethyl)amine Guest Through Multiple Functional Group Interactions[†]

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Characterization Data for Key Compounds:

9: ¹H NMR (CDCl₃) δ 7.7 (s, 1H), 7.2 (broad m, 6H), 6.1-7.1 (broad m, 90 H), 5.4-5.8 (broad m, 32H), 4.5-5.2 (broad m, 48H), 3.7-4.2 (broad s, 64H), 2.1-2.6 (broad s, 64 H); ¹⁹F NMR (TFA internal standard) δ -71.3; MS (MALDI-TOF) 16/16 cross-links calcd. M+Na⁺ = 5219, found M+Na⁺ = 5216, calcd. M+K⁺ = 5235, found M+K⁺ = 5230, 15/16 cross-links calcd. M+Na⁺ = 5247, found M+Na⁺ = 5247; MW_{PS} = 3000.

9-CO₂Me: ¹H NMR (CDCl₃) δ 7.7 (s, 1H), 7.2 (broad m, 6H), 6.1-7.1 (broad m, 90 H), 5.4-5.8 (broad m, 32H), 4.5-5.2 (broad m, 48H), 3.7-4.2 (broad s, 64H), 2.1-2.6 (broad s, 64 H); ¹⁹F NMR (TFA internal standard) δ -70.4; MS (MALDI-TOF) 16/16 cross-links calcd. M+Na⁺ = 5247, found M+Na⁺ = 5250, calcd. M+K⁺ = 5263, found M+K⁺ = 5266, 15/16 cross-links calcd. M+Na⁺ = 5275, found M+Na⁺ = 5279; MW_{PS} = 3200.

14: ¹H NMR (CDCl₃) δ 7.7 (s, 1H), 7.2 (broad m, 6H), 6.1-7.1 (broad m, 90 H), 5.4-5.8 (broad m, 32H), 4.5-5.2 (broad m, 48H), 3.7-4.2 (broad s, 64H), 2.1-2.6 (broad s, 64 H); ¹⁹F NMR (TFA internal standard) δ -71.4; MS (MALDI-TOF) 16/16 cross-links calcd. M+H⁺ = 5196, found M+H⁺ = 5199, calcd. M+Na⁺ = 5219, found M+Na⁺ = 5222, calcd. M+K⁺ = 5235, found M+K⁺ = 5243.

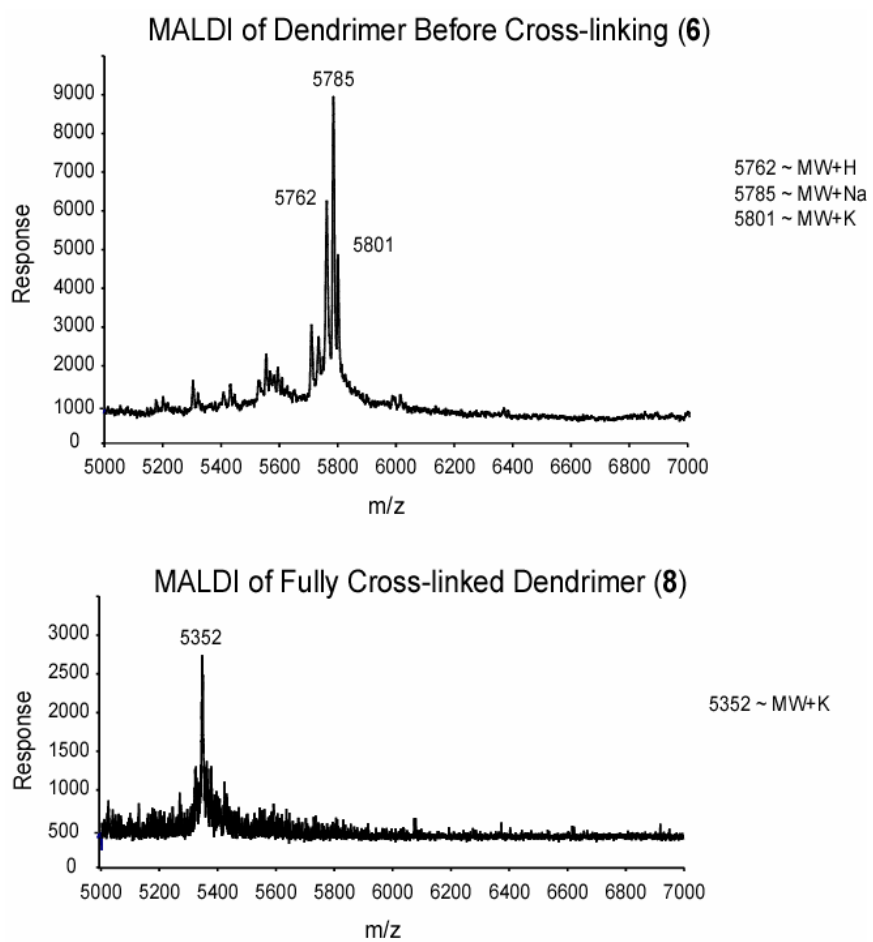


Fig. S1. Representative MALDI-TOF spectra of **6** and **8**.

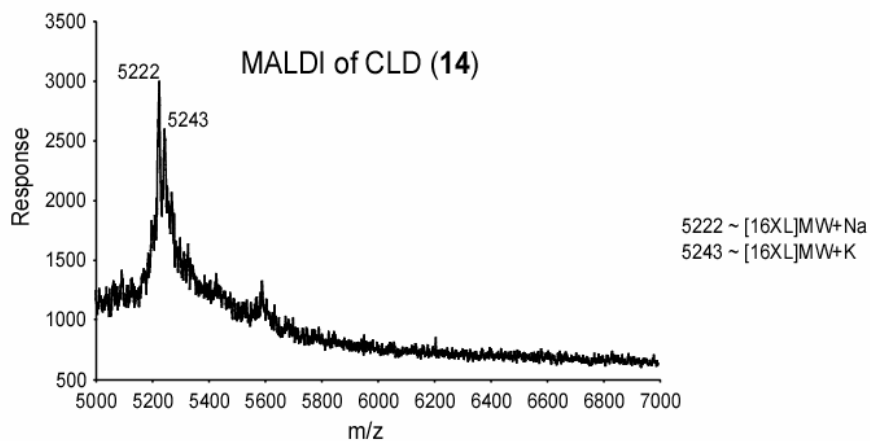
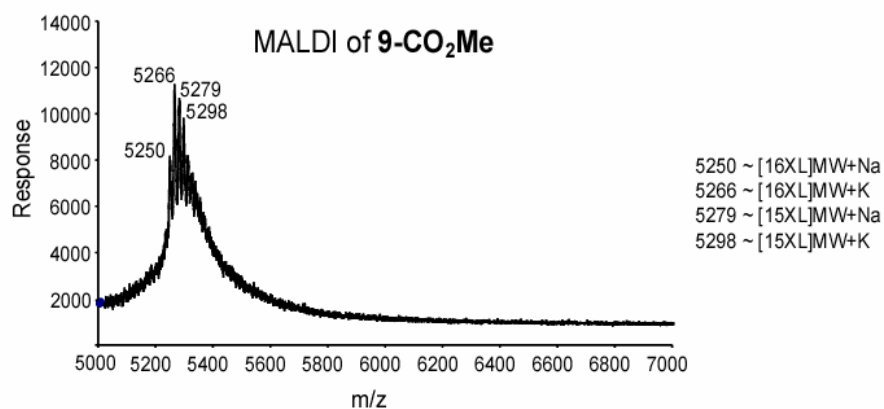
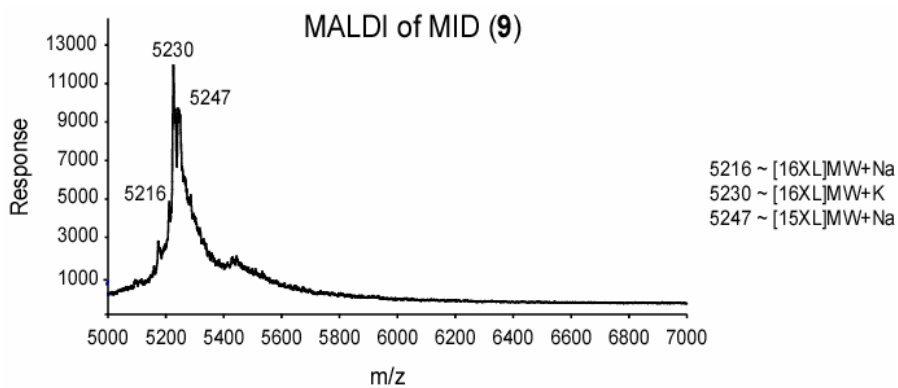


Fig. S2. Representative MALDI-TOF spectra of **9**, **9-CO₂Me**, and **14**.

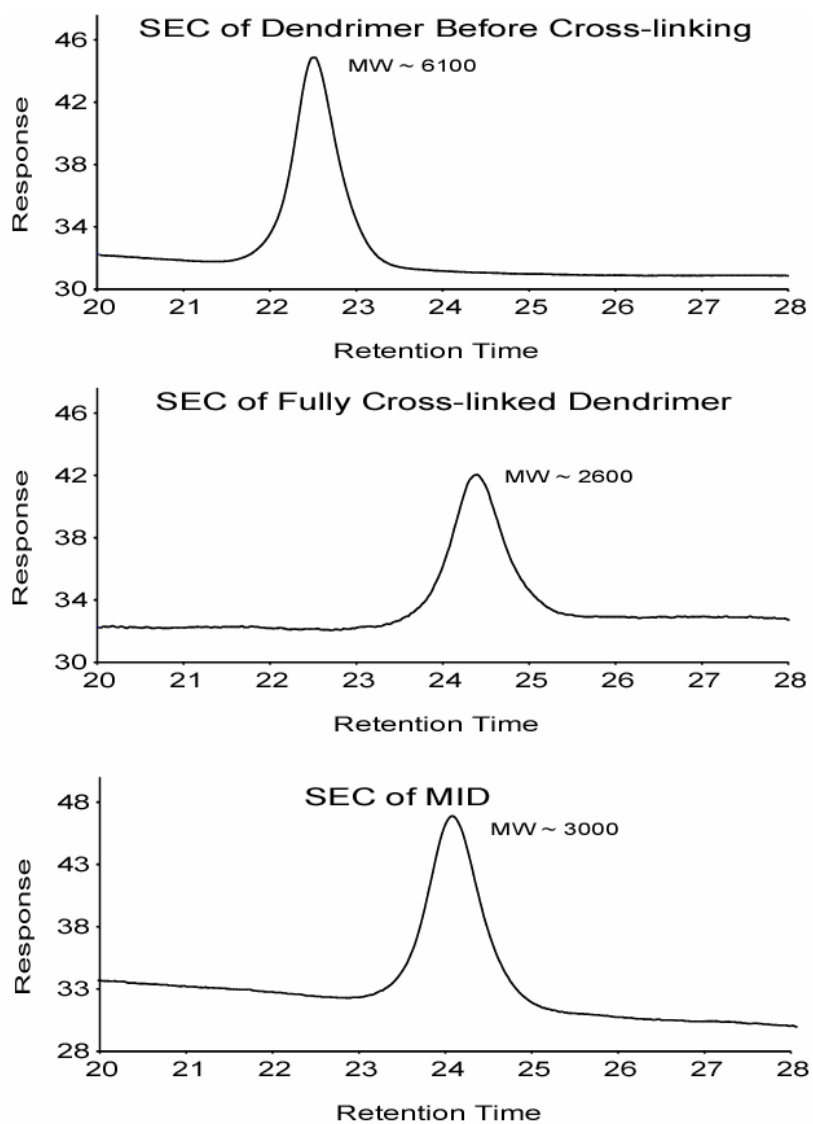
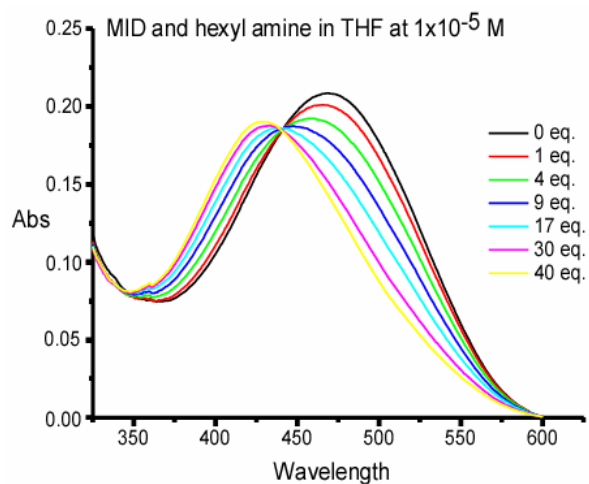
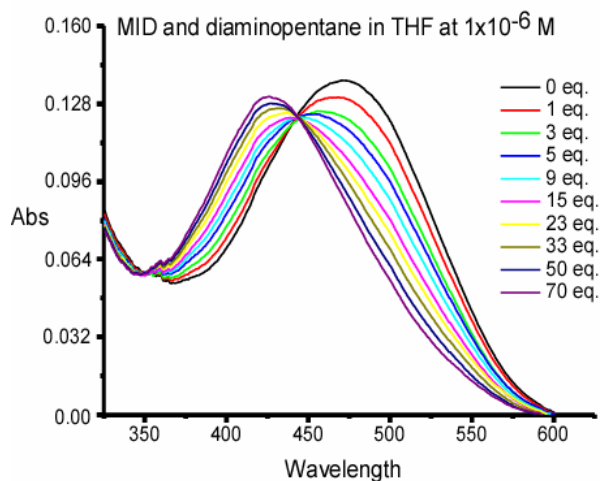


Fig. S3. SEC chromatograms for dendrimers 6, 8, and 9

A.



B.



C.

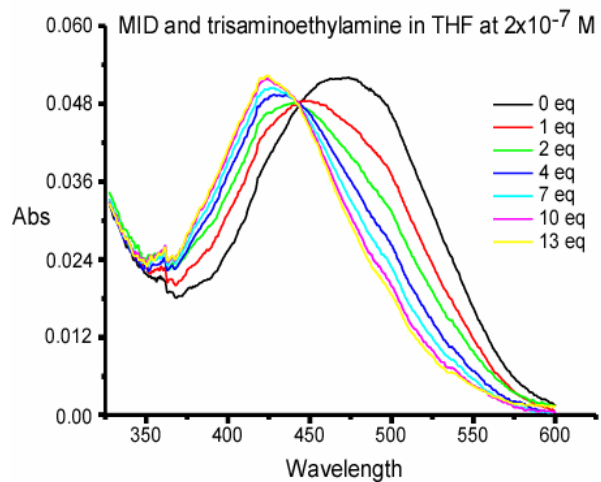
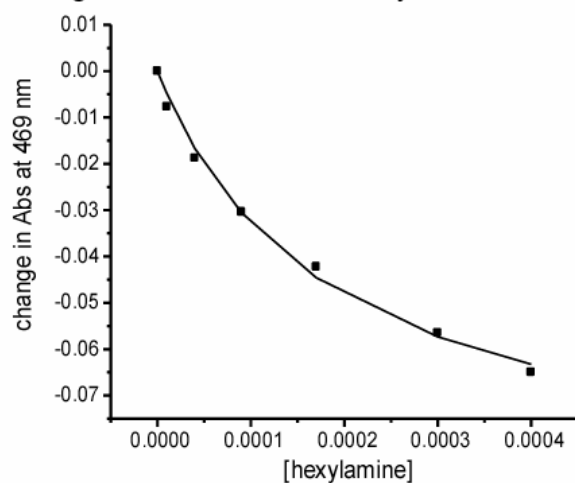


Fig. S4. UV titration curves for MID (**9**) with guests **15** (A), **16** (B), and **4** (C).

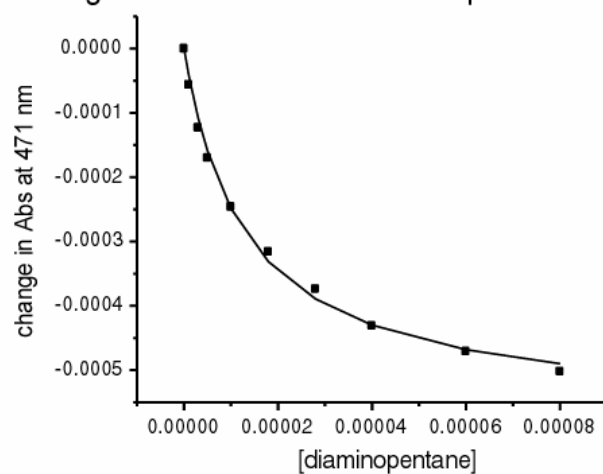
A.

Binding Curve for MID with hexylamine at 1×10^{-5} M



B.

Binding Curve for MID with diaminopentane at 1×10^{-5} M



C.

Binding Curve for MID with trisaminoethylamine at 1×10^{-5} M

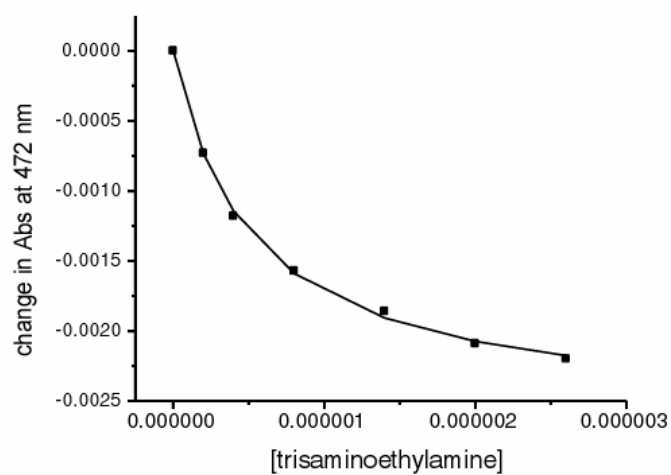


Fig. S5. Binding curves for MID (**9**) with guests **15** (A), **16** (B), and **4** (C).

Table S1. K_{assoc} values for **9**, **9-CO₂Me**, and **14** with simple amine guests^a

Guest	K_{assoc} (M ⁻¹)		
	9-CO₂Me	14	9
CH ₃ (CH ₂) ₅ NH ₂	$(5.7 \pm 0.8) \times 10^3$	N.D.	$(4.5 \pm 1.9) \times 10^3$
H ₂ N(CH ₂) ₅ NH ₂	$(1.1 \pm 0.4) \times 10^4$	$(4.4 \pm 0.8) \times 10^4$	$(2.0 \pm 0.7) \times 10^5$
4	$(1.1 \pm 0.3) \times 10^5$	$(8.0 \pm 3.1) \times 10^5$	$(3.3 \pm 1.1) \times 10^6$

^a Measured in THF at 298 °C. N.D.: Not determined.**Table S2.** ΔG_{298}° values for **9**, **9-CO₂Me**, and **14** with simple amine guests^a

Guest	K_{assoc} (M ⁻¹)		
	9-CO₂Me	14	9
CH ₃ (CH ₂) ₅ NH ₂	5.1	N.D.	5.0
H ₂ N(CH ₂) ₅ NH ₂	5.5	6.3	7.2
4	6.9	8.1	8.9

^a Measured in THF at 298 °C. N.D.: Not determined.