

Partitioning of Poly(amidoamine) Dendrimers between n-Octanol and Water

Supporting Information

Environmental Science and Technology

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Table S1: Selected Physicochemical Properties of the Gx-NH₂ PAMAM Dendrimers Evaluated in This Study

Generation	^a N _{Terminal}	^b M _{wth} (Da)	^c R _H (nm)
G0	4	517	0.96
G1	8	1430	1.18
G2	16	3256	1.47
G3	32	6909	1.86
G4	64	14215	2.44
G5	128	28826	3.12
G6	256	58048	3.81
G8	1024	233383	4.76

^aN_{Terminal}: Number of terminal groups.

^bM_{wth}: Theoretical molar mass.

^cR_H: Hydrodynamic radius. Data are taken from Reference [30]

Table S2: Selected Physicochemical Properties of the G4-X and G3.5 PAMAM Dendrimers Evaluated in This Study.

Generation	Terminal Group	^a N _{Terminal}	^b M _{wth} (Da)
4	^c Amine	64	14215
4	^c Amidoethanol	64	14277
4	^c Succinamic acid	64	20619
3.5	^c Sodium carboxylate	64	26252
4	^c Tris(hydroxymethyl) aminomethane	64	18121
4	^c Pyrrolidinone	64	22285
4	^d Amidoethylethanolamine	64	34492

^aN_{Terminal}: Number of terminal groups.

^bM_{wth}: Theoretical molar mass.

^cEthylenediamine core.

^dDiaminobutane core.

Table S3: Selected Physicochemical Properties of the G4-NH₂ PAMAM Dendrimers Evaluated in This Study.

^a Core	Terminal Group	^b N _{Terminal}	^c M _{wth} (Da)
EDA	Amine	64	14215
DAB	Amine	64	14277
DAH	Amine	64	20619
DAD	Amine	64	26252
Cyst	Amine	64	18121

^aEDA (Ethylene diamine); DAB (Diaminobutane); DAH (Diaminohexane); DAD (Diaminododecane) and Cyst (Cystamine).

^bN_{Terminal}: Number of terminal groups.

^cM_{wth}: Theoretical molar mass.

Figure S1: Experimental setup (slow stirring method) used to measure the logK_{ow} of PAMAM dendrimers.



Figure S2: Typical chromatograms of G_x-NH₂ PAMAM dendrimers with ethylene diamine (EDA) core when injected separately. The injection volume is 25 μ l. The solvent flow rate is 2 mL/min with a gradient of 0-50% ACN (balance water) and UV detection at 210 nm.

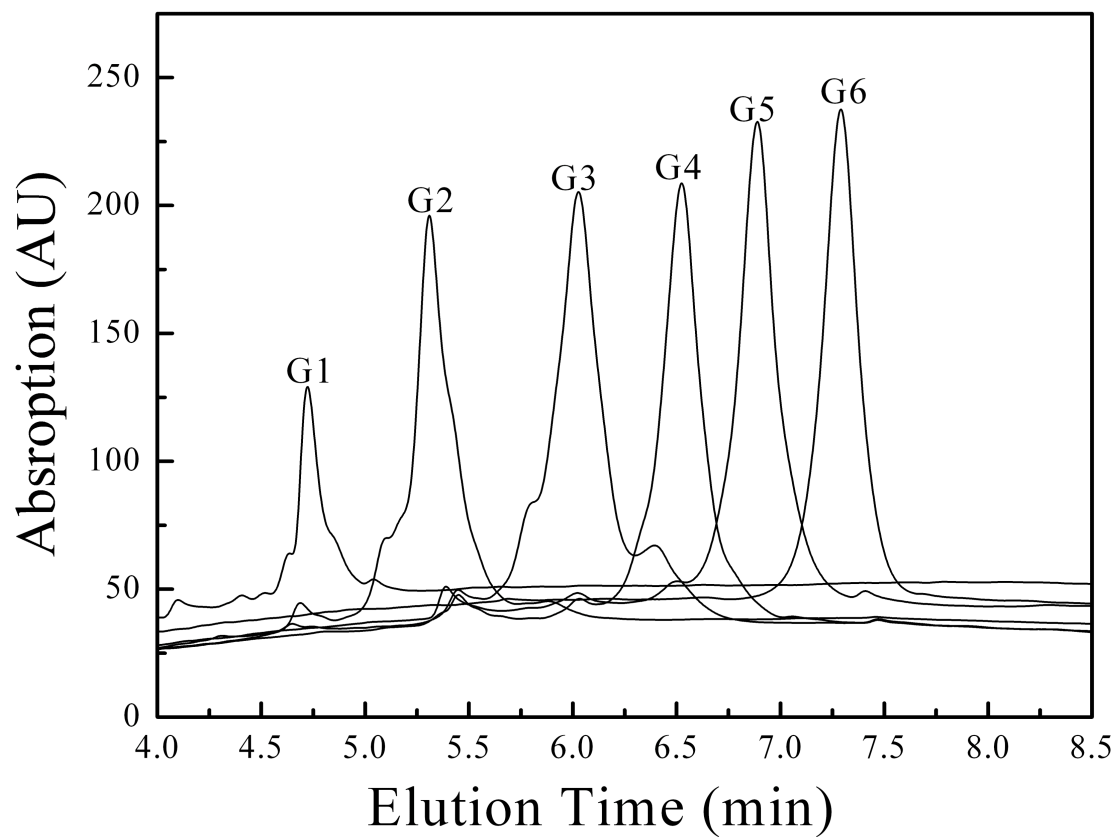
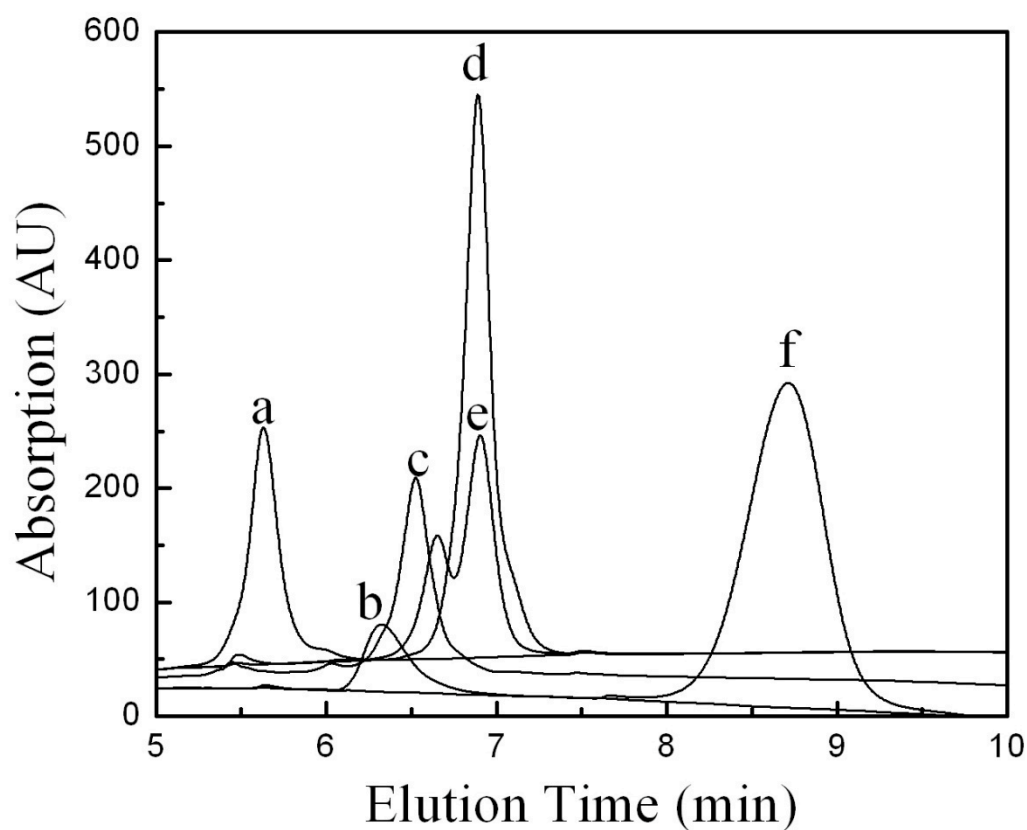


Figure S3: Typical chromatograms of G4 PAMAM dendrimers with ethylene diamine core and different terminal groups when injected separately. a) Tris(hydroxymethyl) aminomethane, b) sodium carboxylate, c) amine, d) succinamic acid, e) amidoethylethanolamine and f) carbomethoxypyrrolidinone. The injection volume is 25 μ L. The solvent flow rate is 2 mL/min with the gradient of 0-50% ACN (balance water) within 15 min. The UV wavelength used for detection is 210 nm.



Figures S4: Typical chromatograms [with INSET calibration curve] used to estimate the $\log K_{ow}$ as illustrated on a G4 PAMAM dendrimer with succinamic acid terminal groups: a) dendrimer peak corresponding to an initial aqueous phase concentration of 36 μM , b) dendrimer peak after equilibrium partitioning between the water and octanol phases, c) standard solution of concentration 30 μM , d) standard solution of concentration 25 μM , e) standard solution of concentration 20 μM , f) standard solution of concentration 10 μM . The injection volume is 25 μL . The solvent flow rate is 2 mL/min with a gradient of 0-50% ACN (balance water) and UV detection at 210 nm.

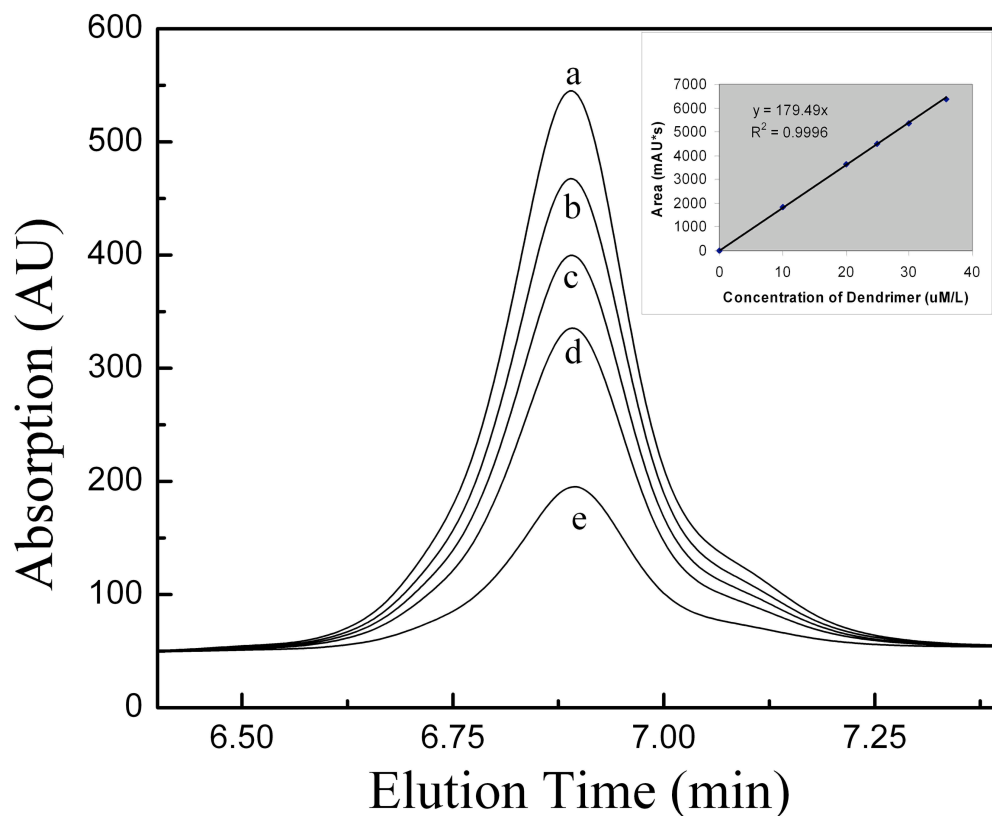


Figure S5: Typical chromatograms of G4 PAMAM dendrimer with succinamic acid terminal groups: a) dendrimer peak corresponding to an initial aqueous phase concentration of $33.72\ \mu\text{M}$ with integrated areas under the peak 6051 ± 6 (counts), b) dendrimer peak after equilibrium partitioning between the water and octanol phases corresponds to dendrimer concentration $33.34\ \mu\text{M}$ with integrated areas under the peak 5985 ± 2 (counts). The injection volume is $25\ \mu\text{l}$. The solvent flow rate is $2\ \text{mL/min}$ with a gradient of 0-50% ACN (balance water) and UV detection at $210\ \text{nm}$.

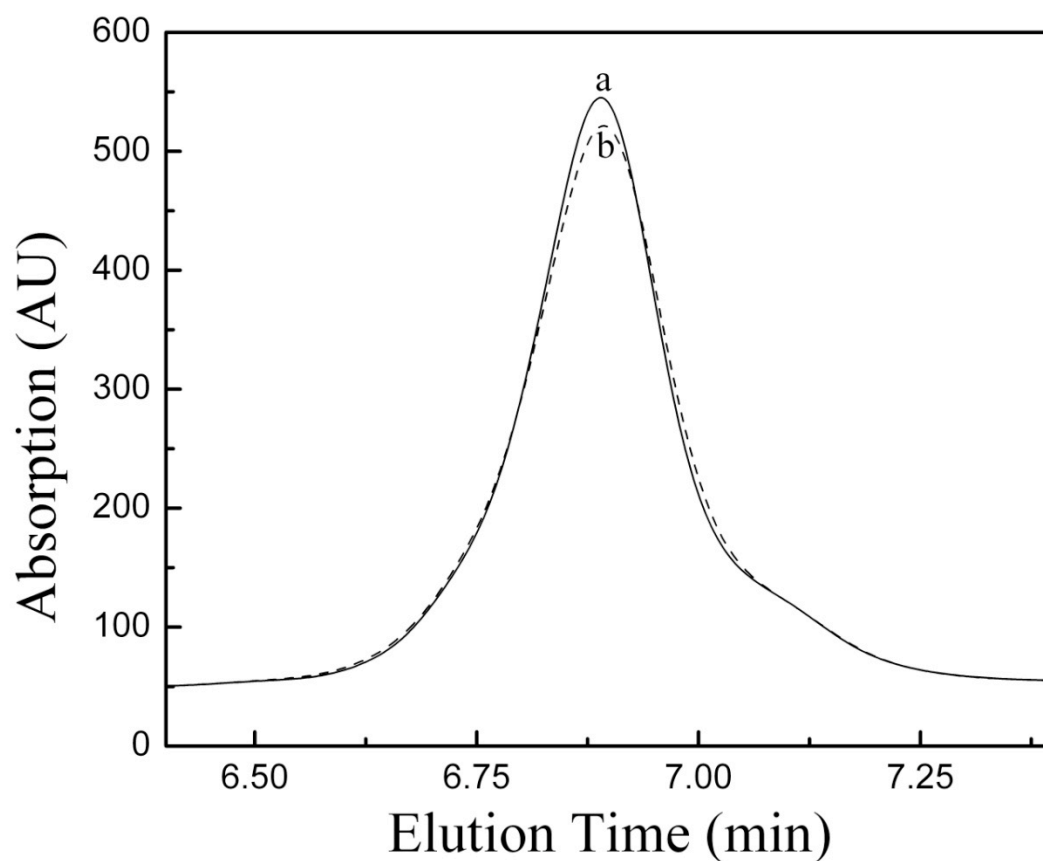


Figure S6: Partitioning of G6-NH₂ PAMAM dendrimer with ethylene diamine core at the octanol-water (O/W) interface. Note that the cloudiness at the O/W interface.

