Supporting Information

PAMAM (starbust) G3, G4 and G5 dendrimers with an ethylenediamine core were purchased from Aldrich Chemical (Milwaukee, WI).

N-(tert-Butoxycarbonyl)-L-phenylalanine (Boc-Phe), *N*-(tert-butoxycarbonyl)-L-leucine (Boc-Leu) and *N*-(tert-butoxycarbonyl)-L-Isoleucine (Boc-Ile) were obtained from Peptide Institute, INC (Osaka, Japan). 1, 3-Dicyclohexylcarbodiimide (DCC) and *N*-hydroxysuccinimide were supplied from Tokyo Kasei Kogyo (Tokyo, Japan). Trifluoroacetic acid, triethylamine, 2-amino-2-hydroxymethyl-1, 3-propanediol (Tris) and N, N-dimethyl formamide (DMF) were from Kishida Chemical (Osaka, Japan). Dimethyl sulfoxide (DMSO) and ethidium bromide were from Wako Pure Chemical Industries (Osaka, Japan).

PAMAM dendrimers having Phe and Leu residues were prepared as previously reported [6]. Ile-(G4) dendrimer was prepared by the same procedure. Yiels: 30.3 mg, 35.0%. ^{1}H NMR: 400MHz; D2O; Me4Si0.73 and 0.76 (384 H, br s, CH3 in Ile), 1.06 and 1.29 (128 H, br s, CHCH2CH3 in Ile), 1.63 (64 H, br s, CHCH2CH3 in Ile), 2.28 (248 H, br s, CH2CH2CONHCH2CH2N in PAMAM), 2.49 (248 H, br s, CH2CH2CONHCH2CH2N in PAMAM), 2.68 (248 H, br s, CH2CH2CONHCH2CH2N

in PAMAM), 3.19 (376 H, br m, CH2CH2CONHCH2CH2NH2 in PAMAM), 3.29 (64 H, br s, CαH in Ile).

The numbers of Phe and/or Ile residues at the dendrimer periphery were evaluated from the integral ratios of the signals at 7.1-7.2 ppm (Phe), 0.9 ppm (Ile), and 2.2 ppm (PAMAM dendrimer) in ^{1}H NMR spectra of the dendrimers having Phe and/or Ile residues. ^{1}H NMR spectra for the PAMAM dendrimers having Phe and Ile residues were shown in Figure S-1.

The transmittance at 600 nm was measured using Jasco Model V-550 spectrophotometer. The heating rate was adjusted at 1.0 ^{o}C/min using ETC-505T apparatus (Jasco).

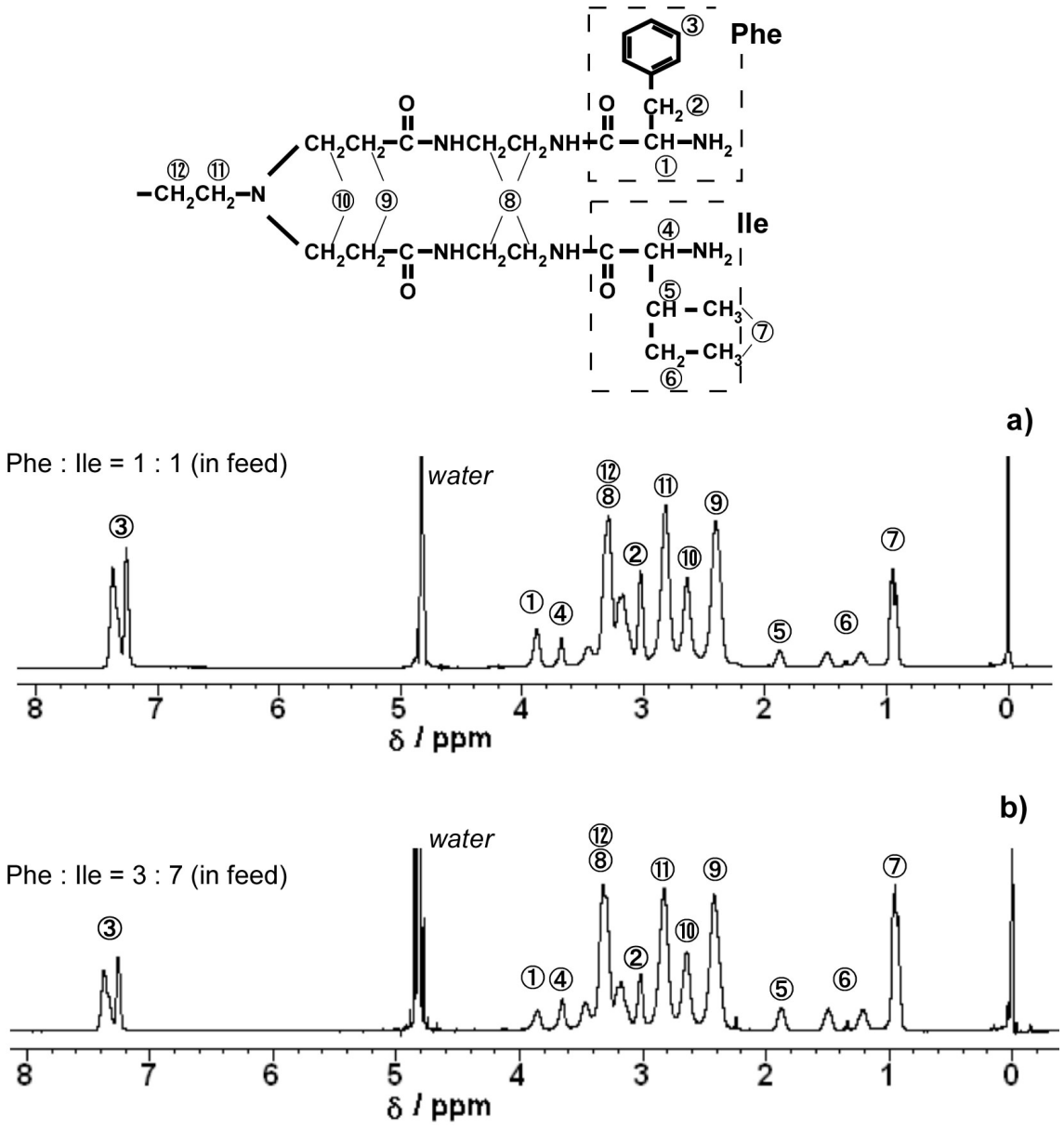
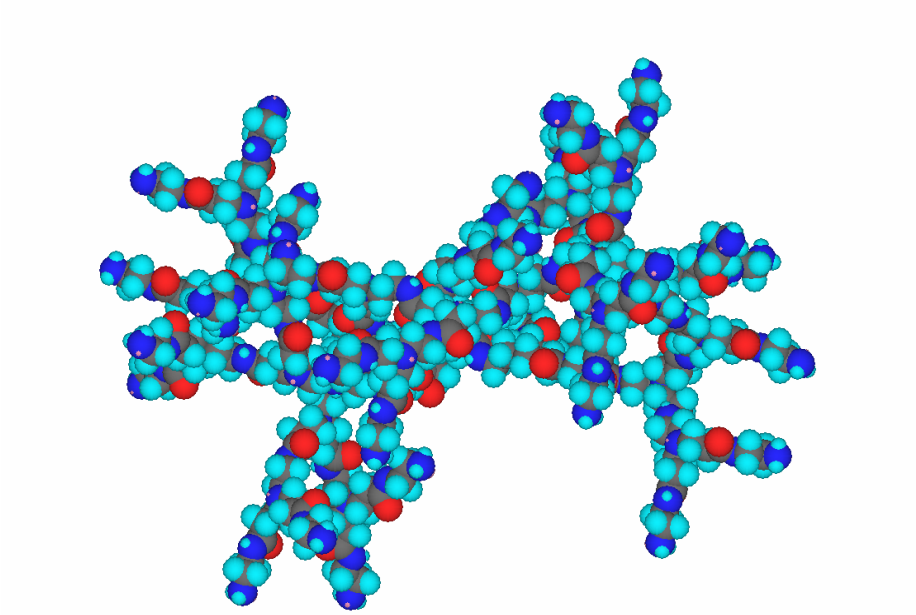
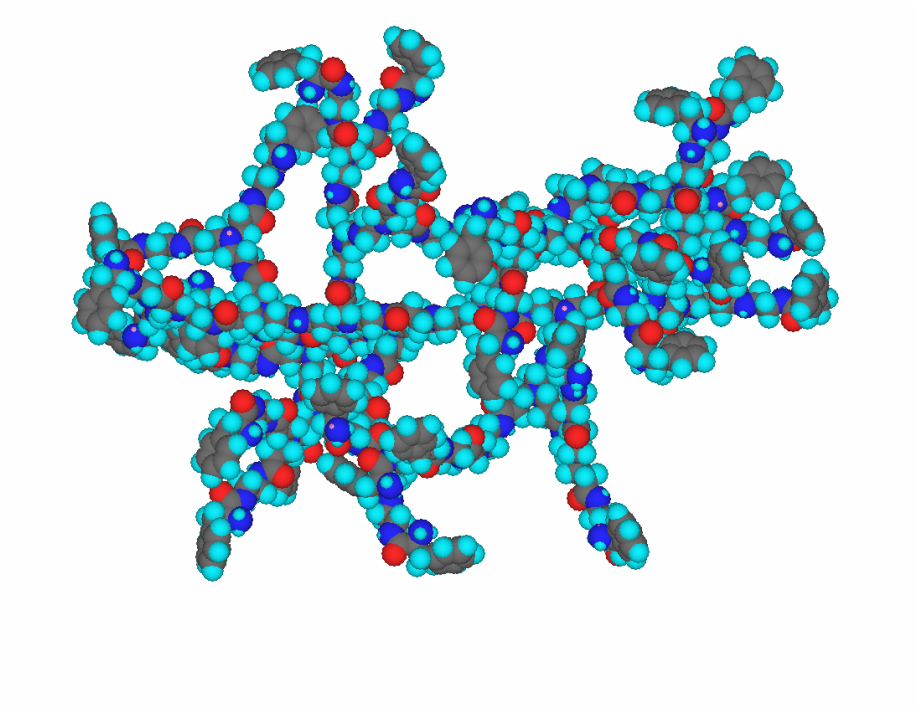


Fig. S-1. ^{1}H NMR spectra of Phe$_{44}$-Ile$_{20}$-G4 (a) and Phe$_{30}$-Ile$_{33}$-G4 (b) in D_2O.

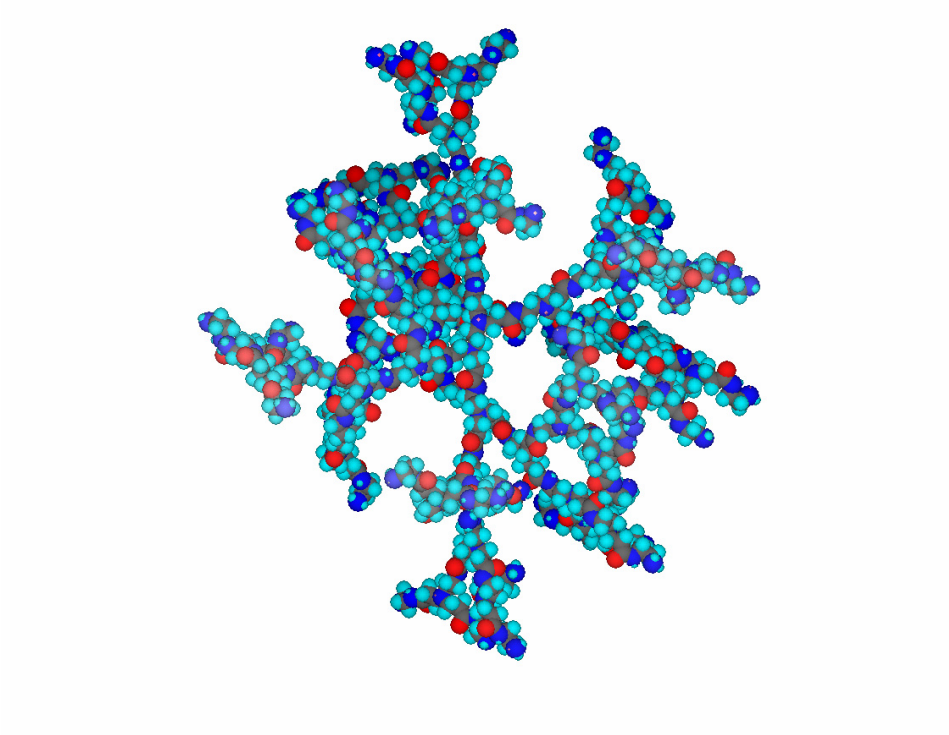
The low-energy conformers of dendrimers obtained using Chem3D software.



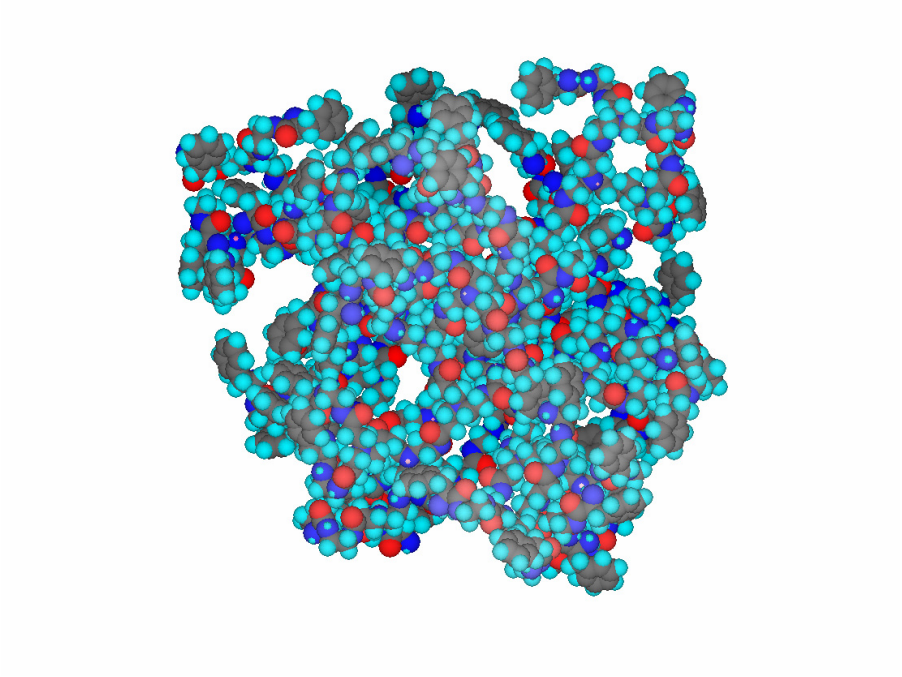
G3 dendrimer



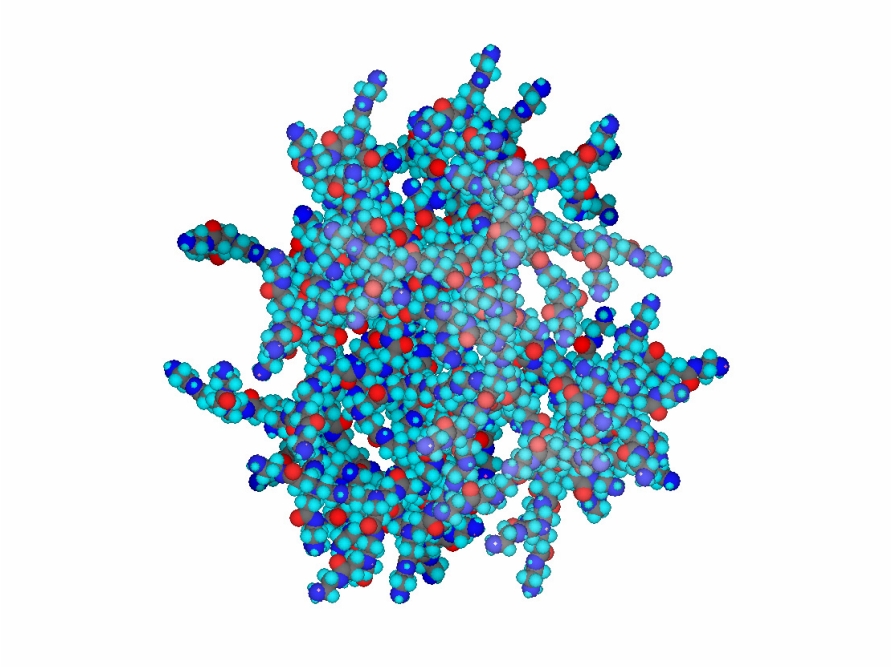
G3-Phe dendrimer



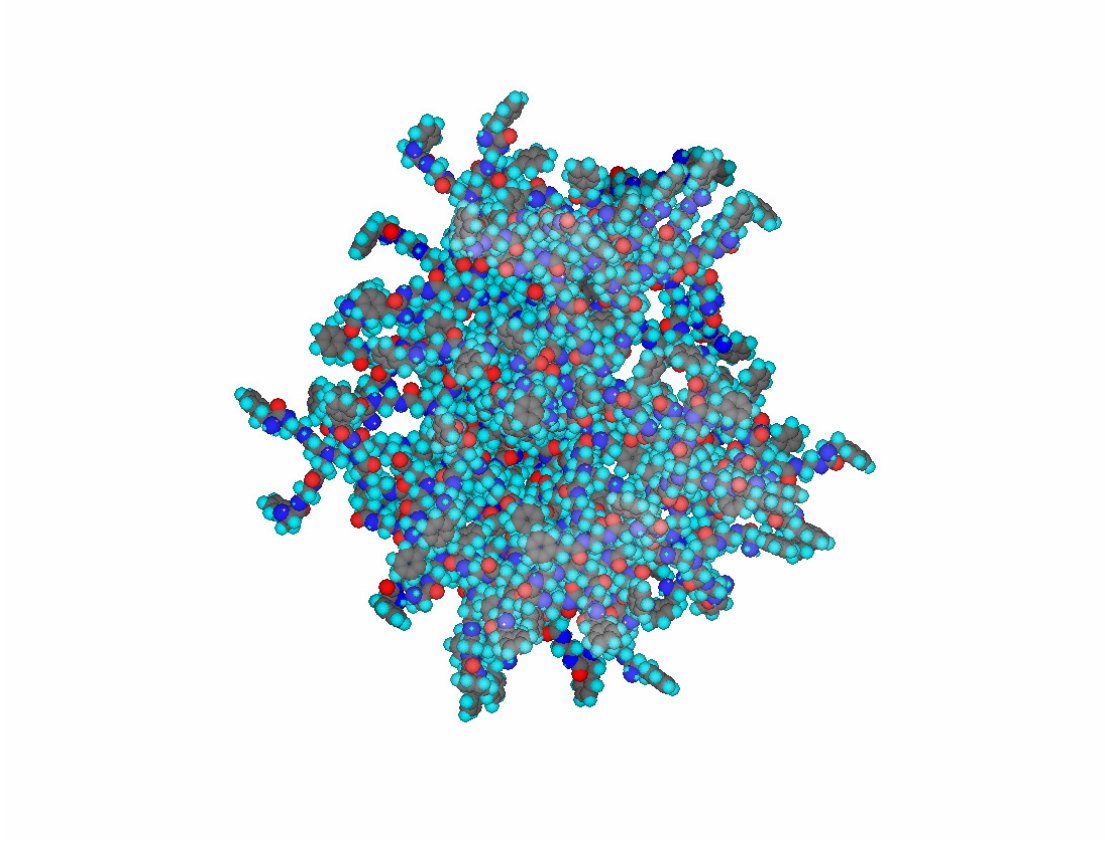
G4-dendrimer



G4-Phe dendrimer



G5 dendrimer



G5-Phe dendrimer