Supporting Information for:

Bi-functional Polyamines for the Aqueous Dispersion of Carbon Nanotubes and Formation of CNT-Impregnated Hydrogel Composites

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Experimental Section:

Chemicals and Supplies

Chemicals, including 1-bromobutane, 1-bromooctane, 1-bromododecane, benzyl bromide, 1-(bromomethyl)-3,5-dimethoxybenzene, 1-(bromomethyl)-3,5-difluorobenzene, HCl, and poly(2-ethyloxazoline) were purchased from Sigma-Aldrich and used as received. LPEI was synthesized by the acidic hydrolysis of poly(2-ethyloxazoline) as previously reported.[1]

Hydrophobic Modification of LPEI

LPEI (0.2 g) was dissolved into a heated solution of 10:1 acetonitrile and methanol, an appropriate amount of the alkyl bromide was added (0.2 molar equivalents relative to LPEI), and the mixture was heated to reflux solvent overnight. The solvent was evaporated under reduced pressure, and the products were washed with hexanes to remove any unreacted alkyl bromides. Yields were 95% or greater, and the polymers were used without further purification.

^{1}H NMR Characterization of the Polymers

NMR spectra were taken on a Bruker Avance^{tm} 400 MHz multinuclear NMR (Bruker, Billerice, MA) in CD_3OD. To measure the amount of substitution for each polymer, the peaks from the tether were integrated appropriately and the relative area under the polymer backbone peaks was used to calculate the substitution percentage, similarly to the characterization of ferrocene-modified LPEI as reported previously.[2] All polymers had a substitution percentage of 22 ±2%. The NMR spectra for the polymers are shown below in Figures S1-S6.

Optical Density measurements for the characterization of CNT dispersion

All examples of previously mentioned hydrophobically modified LPEI samples were dissolved at concentrations of 250 mM and adjusted to pH 1 by addition of 6 M hydrochloric acid. When fully dissolved, the individual solutions were added to samples of single-wall carbon nanotubes (length- 0.5-2 mm, o.d. 1-2 mm and > 90% purity) (Cheaptubes.com) to result in a 1 mg/mL suspension of carbon nanotubes in a given polymer solution. Each sample was vortexed for approximately 30 seconds and sonicated for 2 minutes using a microtip ultrasonic probe (Fisher Scientific sonic dismembranor Model 100). After sonication, all samples were centrifuged at 5000 x g for 10 minutes to separate out agglomerations of SWCNTs and allow for only dissolved or fully suspended SWCNTs to remain in the supernatant. A 1 to 10 dilution of each SWCNT suspension supernatant was made in 18 MΩ deionized water. Absorbance spectra were obtained for each polymer solution from 300 to 900 nm to ensure no significant electronic transitions at 600 nm (Shimadzu UV-2501PC UV-Vis). Then, a 1 to 10 dilution of each of the polymer solutions was also made containing no nanotubes to zero the absorbance reading of the instrument at 600 nm for each polymer. Absorbance readings were then taken at 600 nm for each sample of carbon nanotube suspension supernatant after the 1 to 10 dilution. This experiment was performed in triplicate for each polymer/nanotube solution.

References

(1) York, S.; Frech, R.; Snow, A.; Glatzhofer, D. *Electrochemica Acta* **2001**, *46*, 1533.
(2) Merchant, S.; Meredith, M. T.; Tran, T. O.; Brunski, D.; Johnson, M. B.; Glatzhofer, D. T.; Schmidtke, D. W. *J. Phys. Chem. C* **2010**, *114*, 11627.

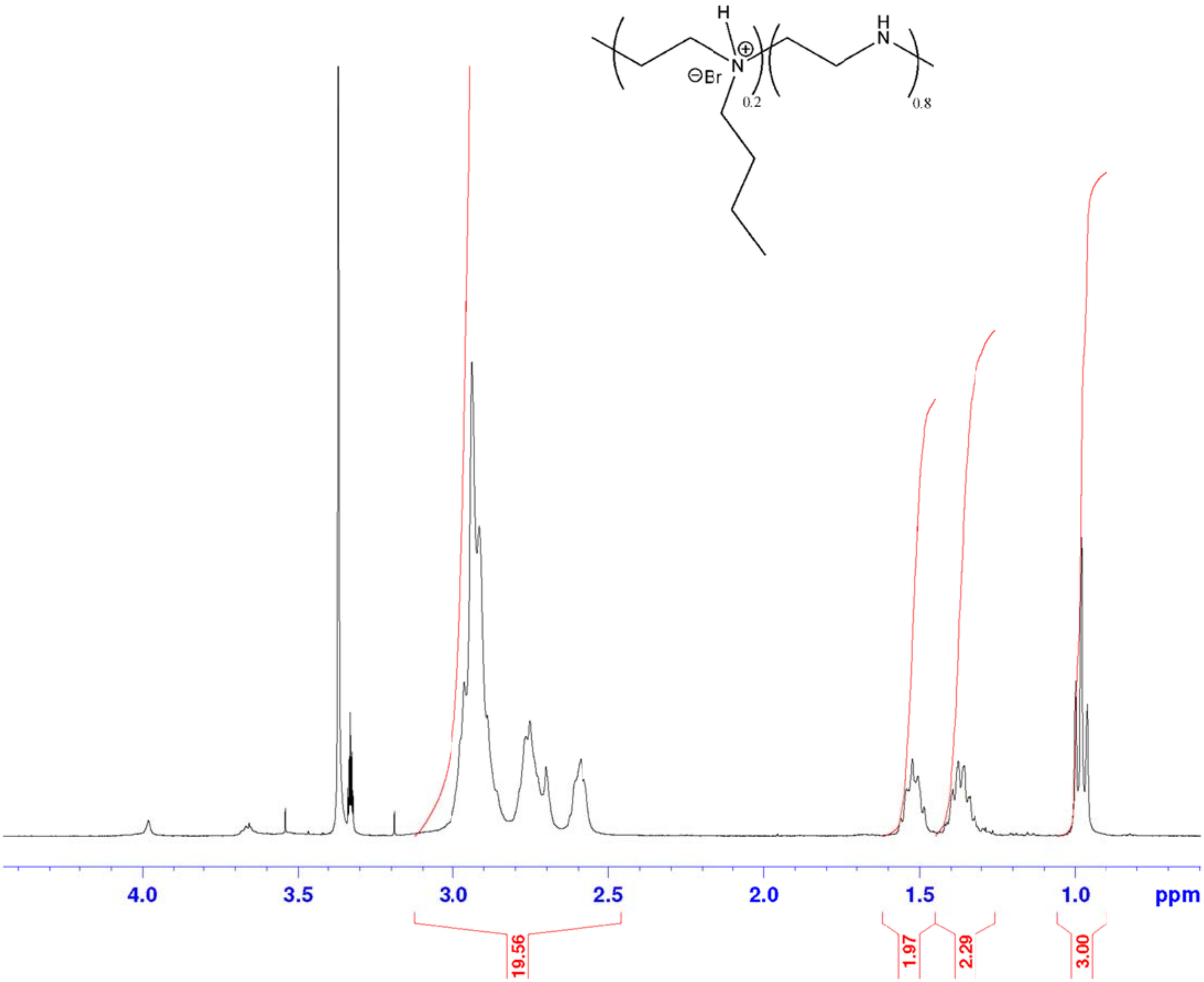

Figure S1: NMR Spectrum of LPEI-C4

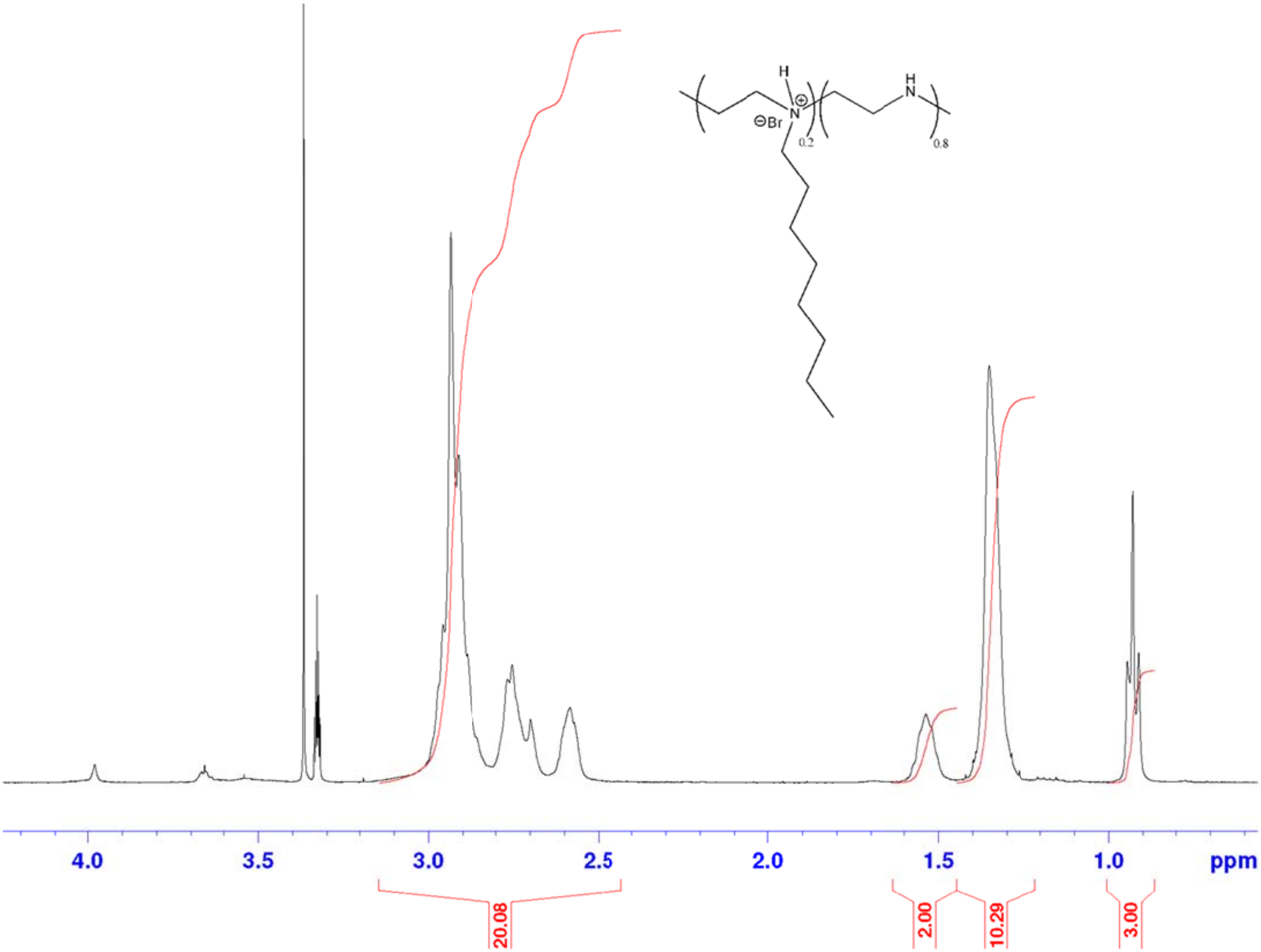

Figure S2: NMR Spectrum of LPEI-C8

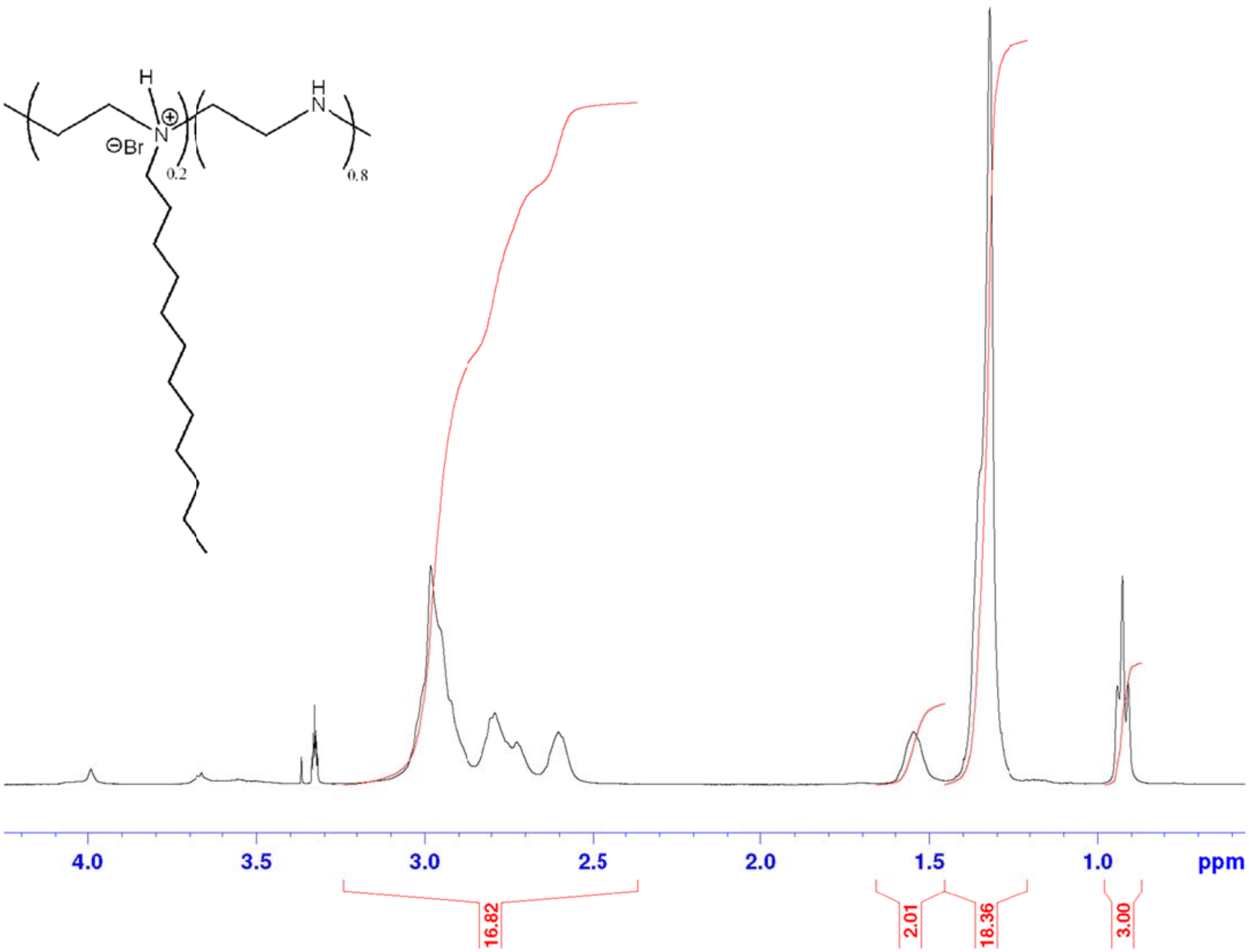

Figure S3: NMR Spectrum of LPEI-C12

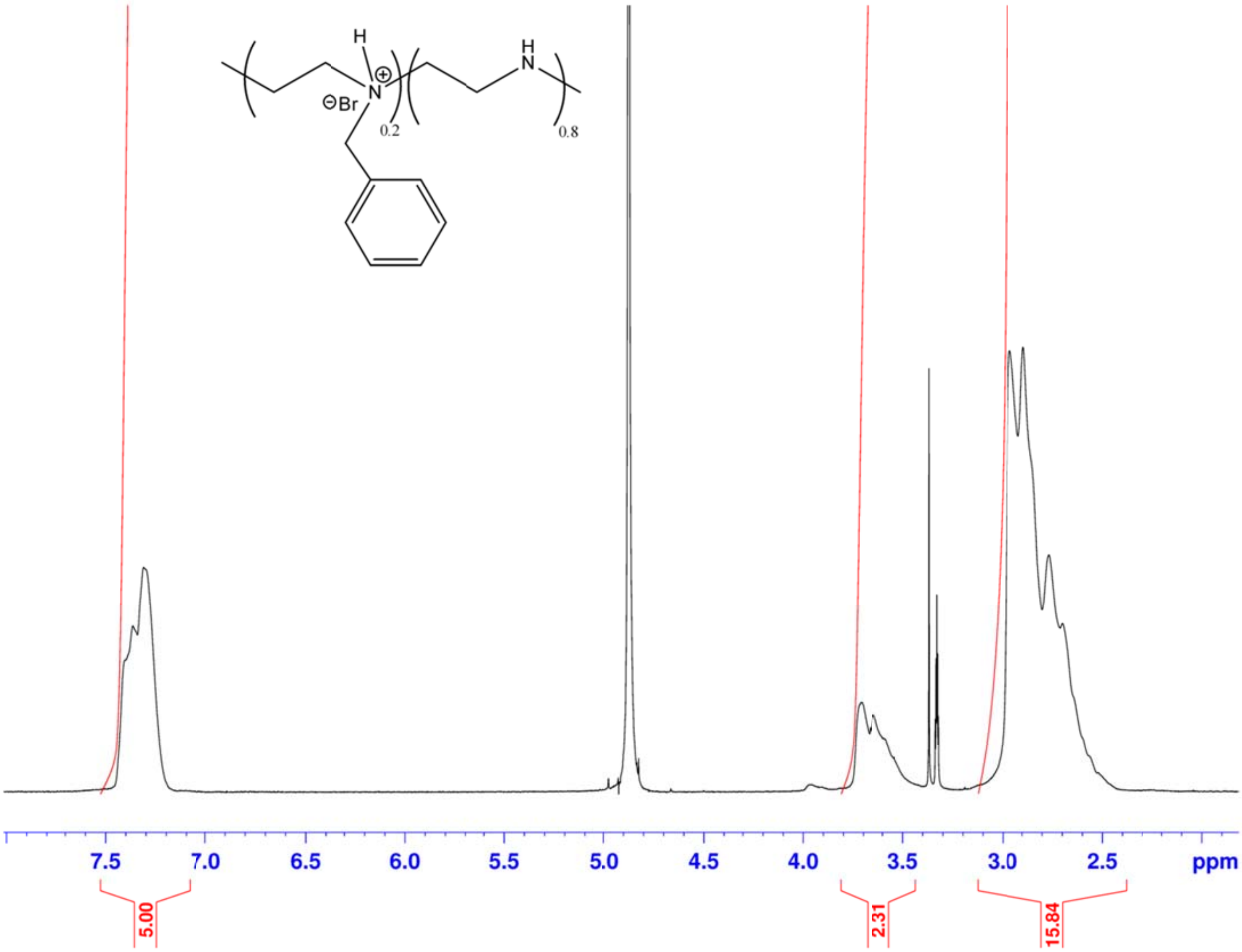

Figure S4: NMR Spectrum of LPEI-Bn

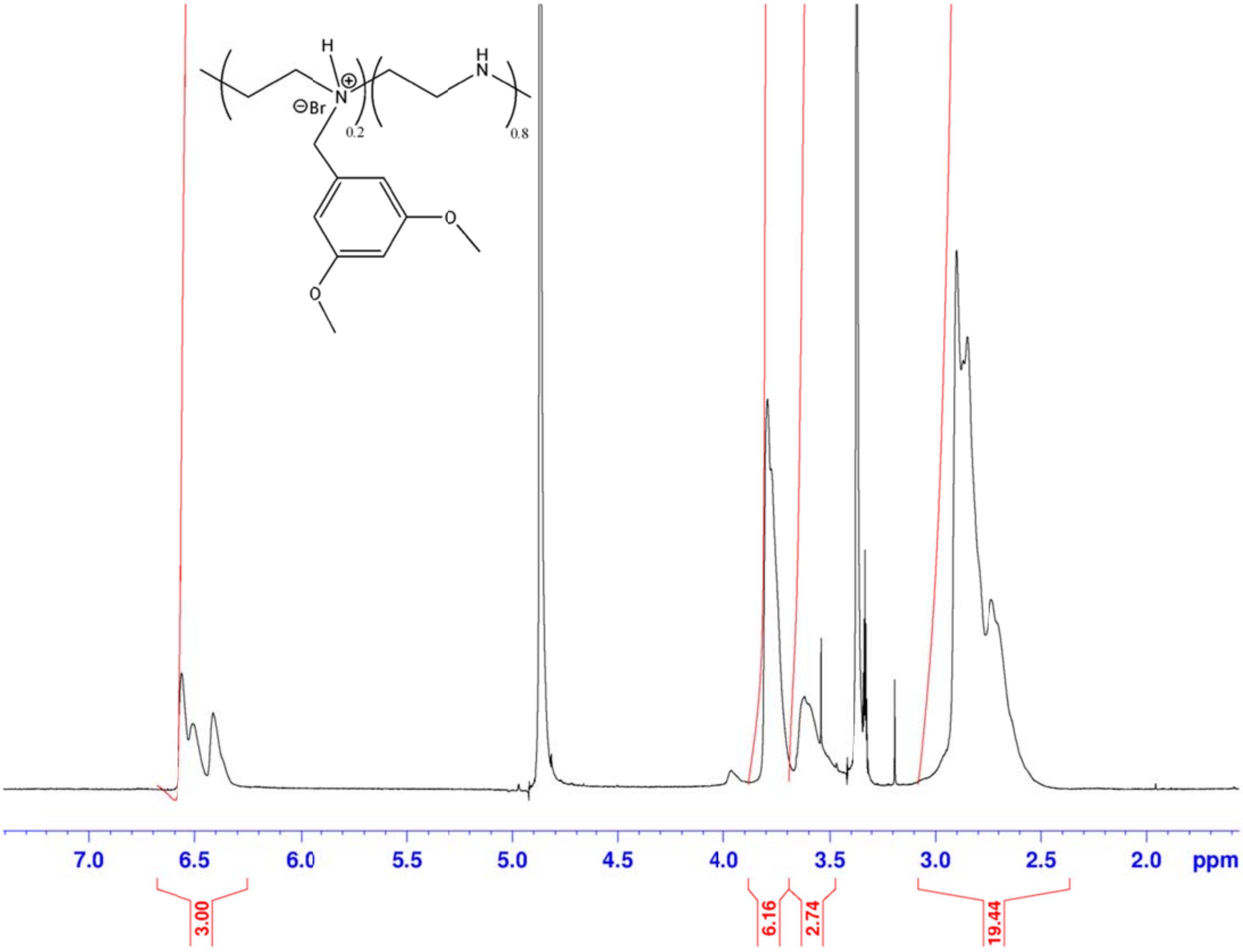

Figure S5: NMR Spectrum of LPEI-Bn(OMe)$_2$

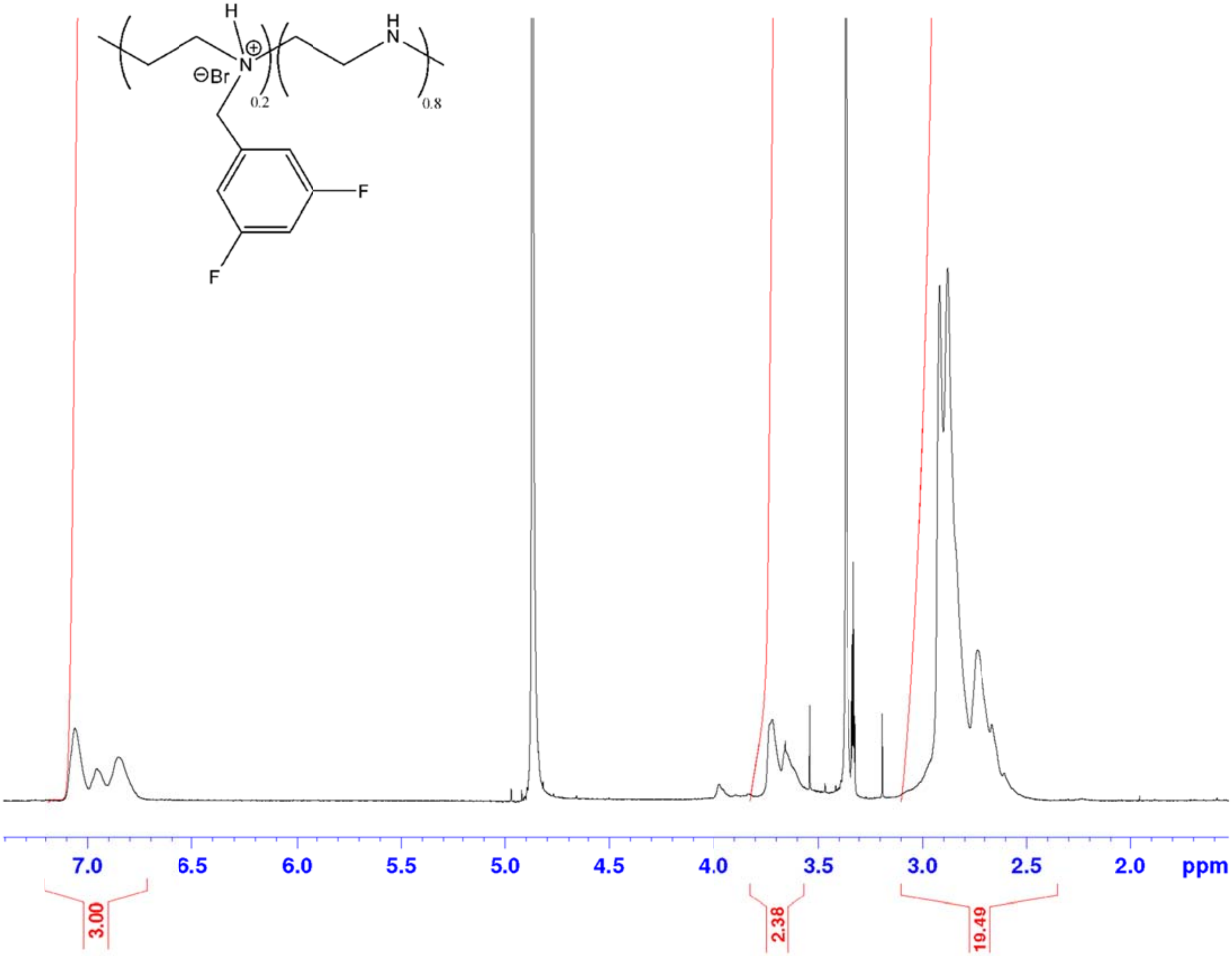

Figure S6: NMR Spectrum of LPEI-BnF$_2$

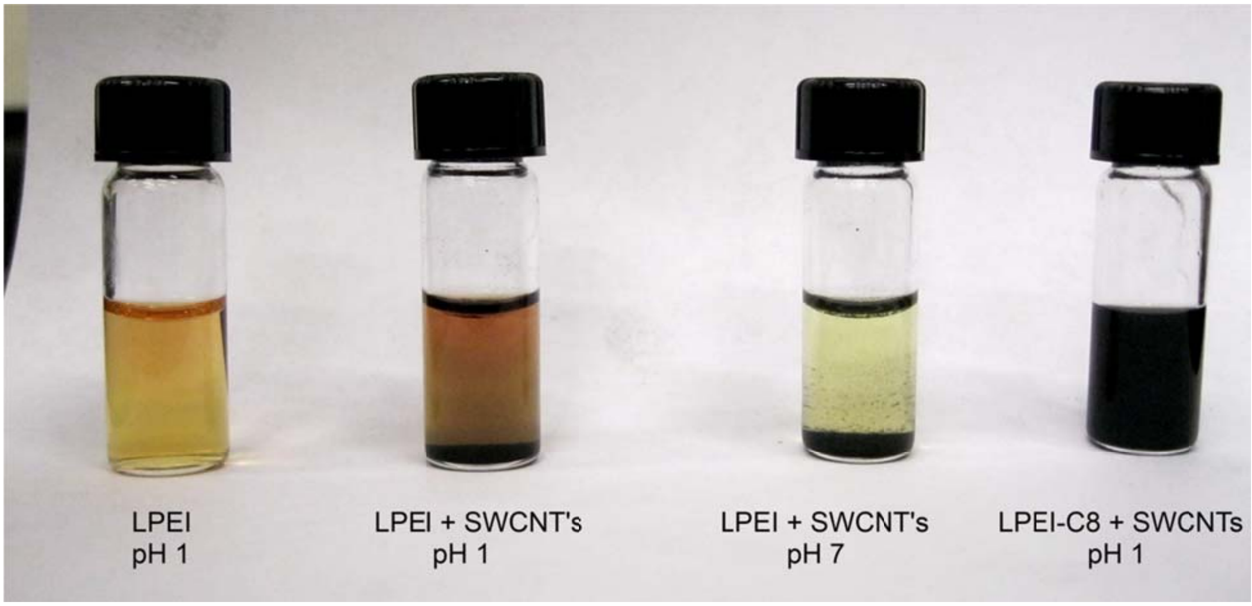

Figure S7: Relative comparison of SWCNT dispersions in LPEI samples. 250 mM polymer, 1 mg/mL SWCNT's. Samples were dissolved in water with HCl, and the pH was adjusted accordingly with NaOH. SWCNT's were added and the solution was sonicated for 10 min. followed by 24 hrs. of stagnation before photographs were taken.