Electronic Supplementary Information for:

Systematic Structure Control of Ammonium Iodide Salts as Feasible UCST-type Forward Osmosis Draw Solutes for the Treatment of Wastewater

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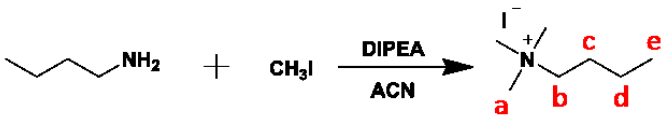
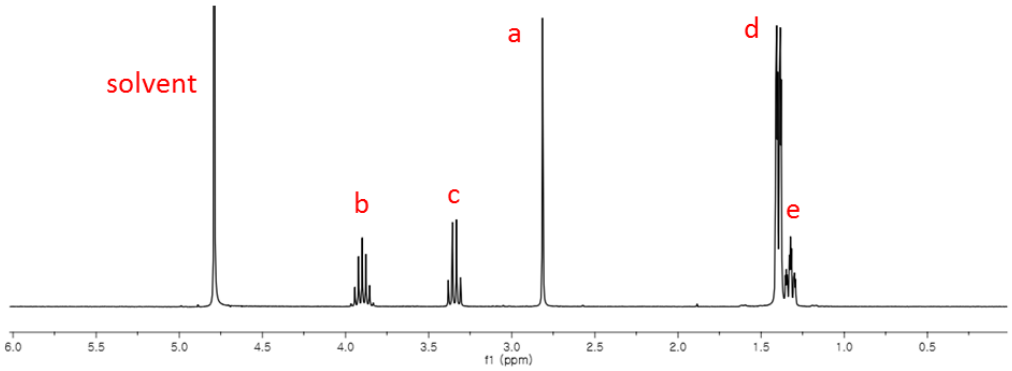
Table of contents:

a)



3MBAI



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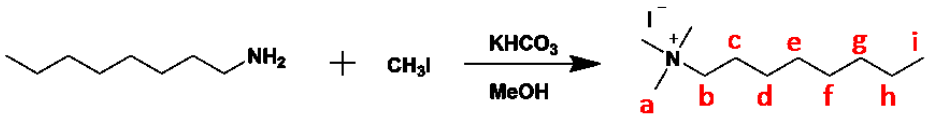

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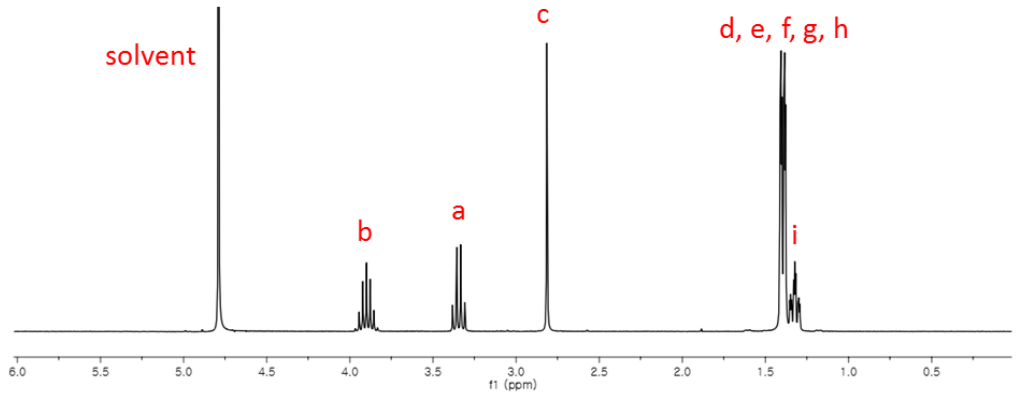

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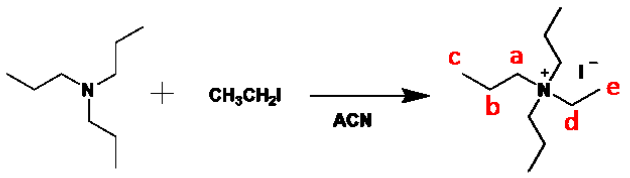

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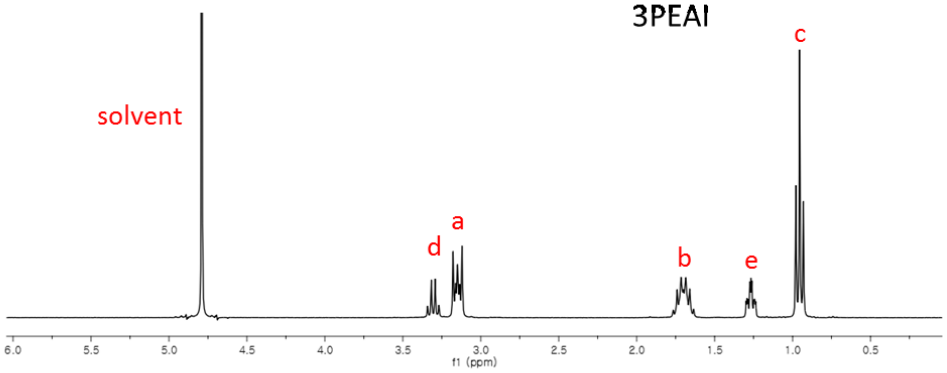

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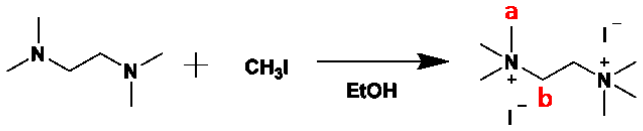
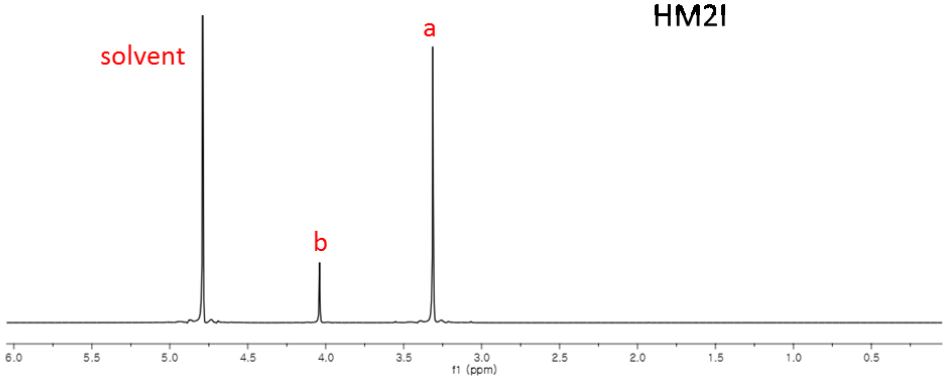


HM2I



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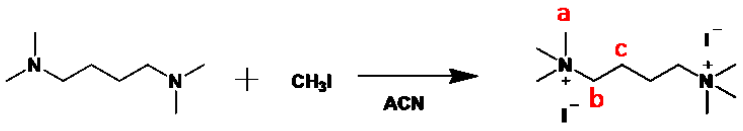

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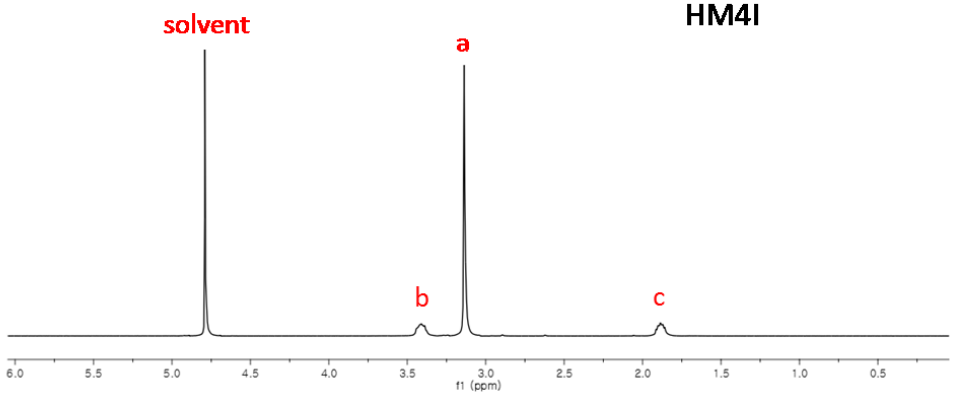

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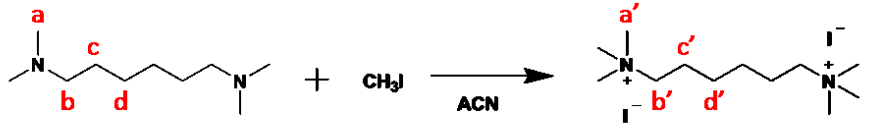
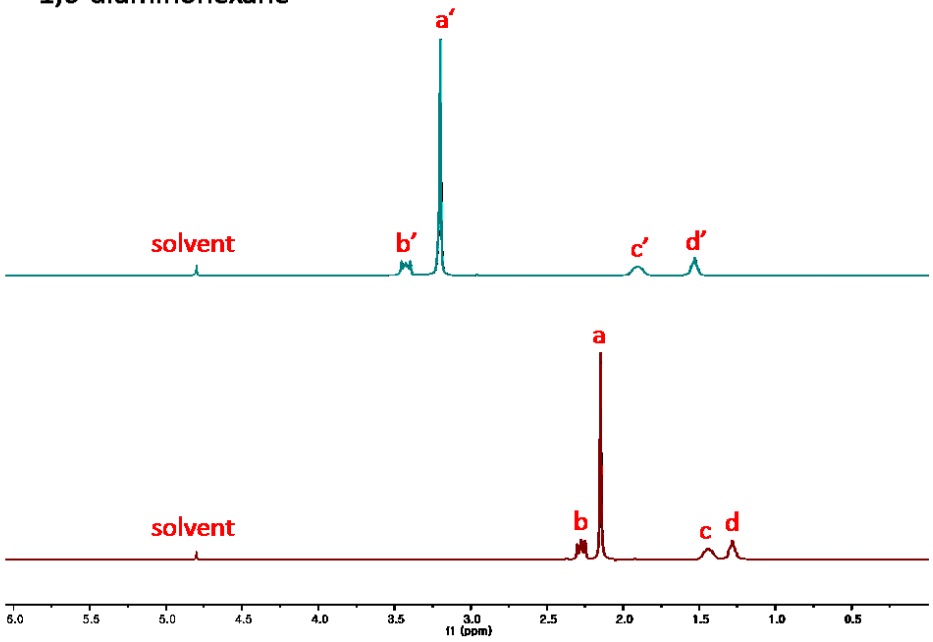


N,N,N′,N′-Tetramethyl
-1,6-diaminohexane

HM6I



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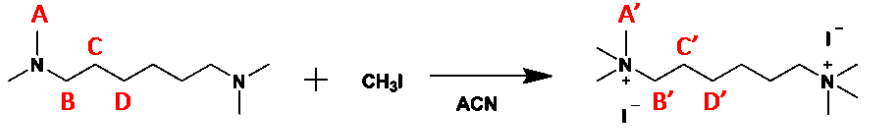
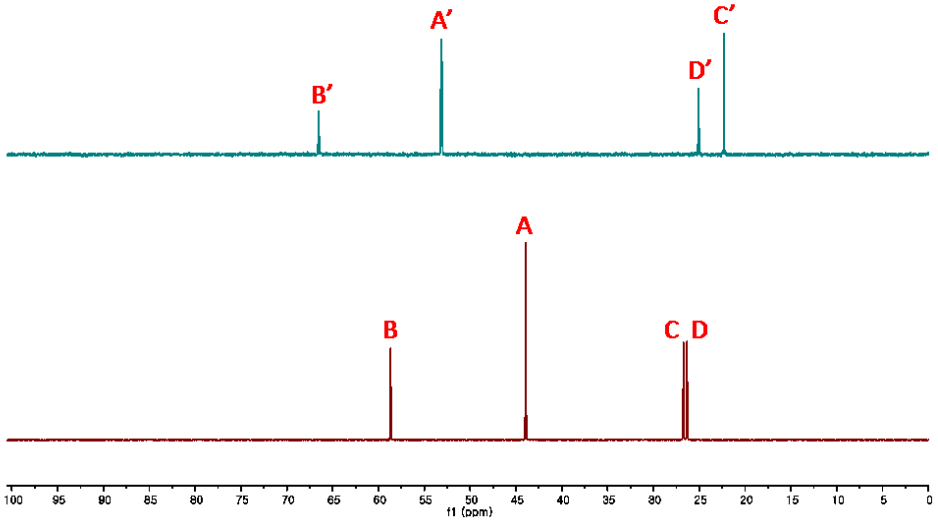


N,N,N′,N′-Tetramethyl
-1,6-diaminohexane

HM6I



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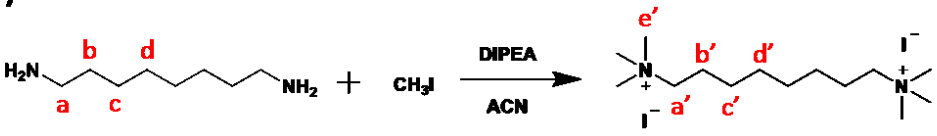
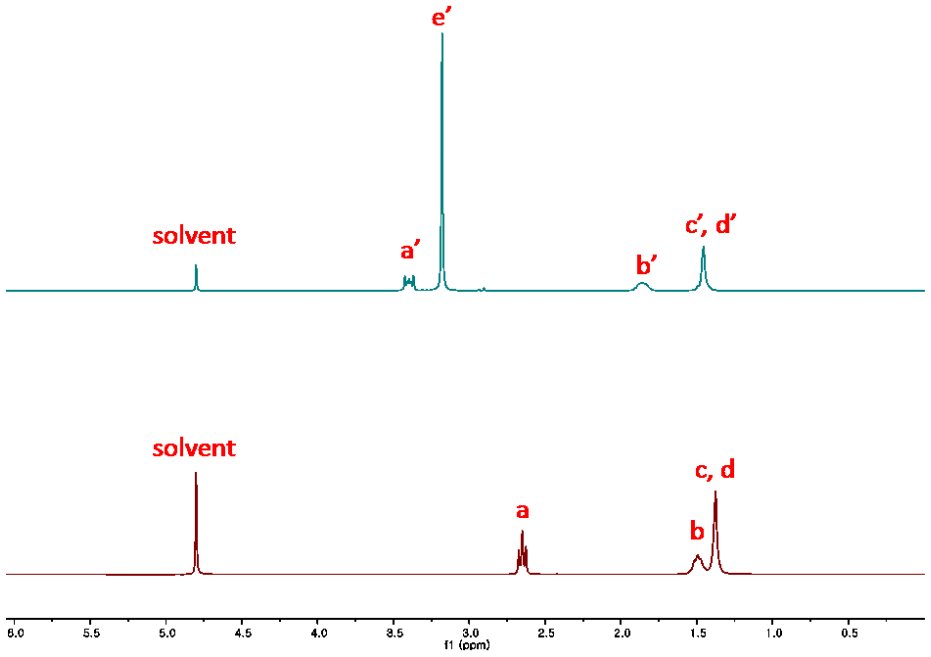


1,8-Diaminooctane HM8I



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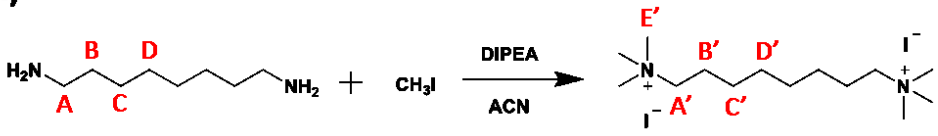
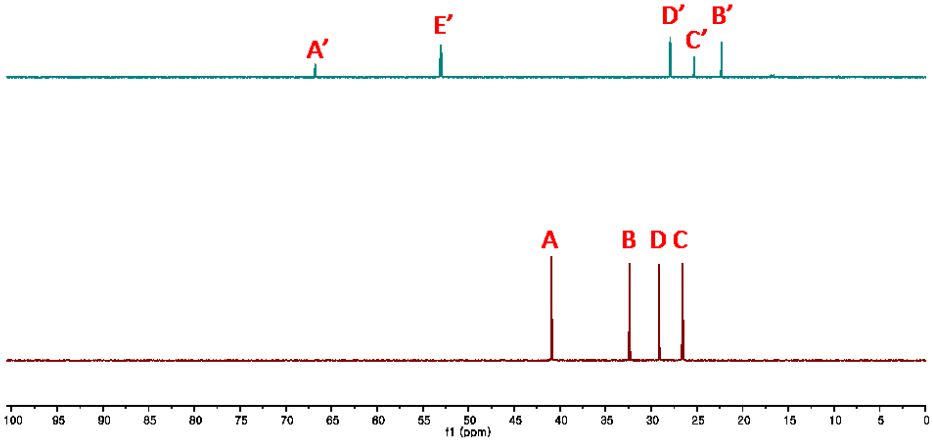


1,8-Diaminooctane HM8I



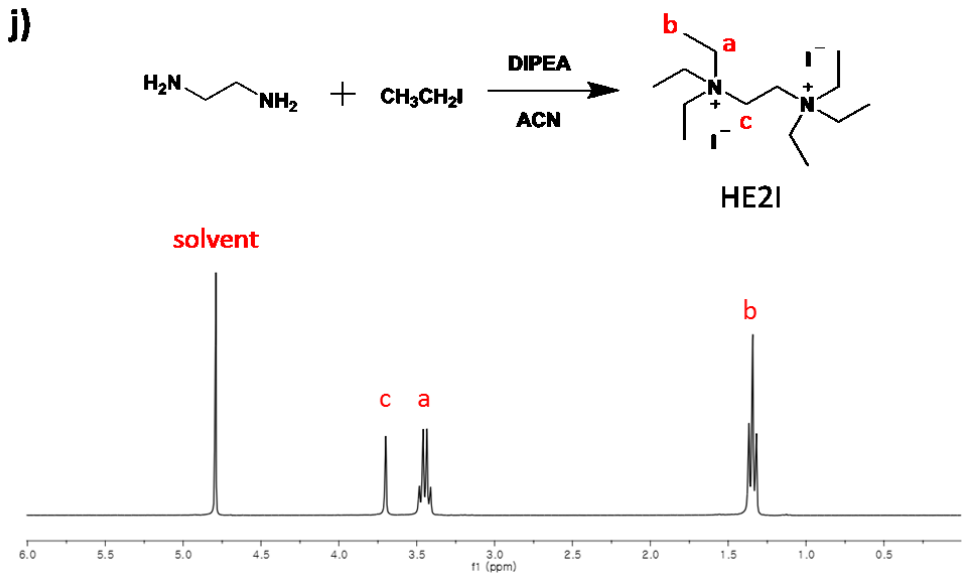


Figure S1. Synthetic scheme and ^{1}H NMR spectra of a) 3MBAI (^{1}H NMR (300 MHz, D_2O, δ): 3.90 (hept, J = 6.6 Hz, 1H), 3.34 (q, J = 7.4 Hz, 1H), 2.81 (s, 1H), 1.45 – 1.36 (m, 6H), 1.36 – 1.27 (m, 2H)), b) 3MOAI (^{1}H NMR (300 MHz, D_2O, δ): 3.37 – 3.26 (m, 1H), 3.11 (s, 4H), 1.86 – 1.70 (m, 1H), 1.36 (d, J = 3.5 Hz, 2H), 1.29 (s, 3H), 0.87 (dd, J = 8.8, 4.8 Hz, 1H)), c) 3PEAI (^{1}H NMR (300 MHz, D_2O, δ): 3.30 (q, J = 7.3 Hz, 1H), 3.21 – 3.09 (m, 3H), 1.79 – 1.60 (m, 3H), 1.33 – 1.20 (m, 1H), 0.95 (t, J = 7.3 Hz, 4H)), d) HM2I (^{1}H NMR (300 MHz, D_2O, δ): 4.04 (s, 1H), 3.31 (s, 4H)), e) HM4I (^{1}H NMR (300 MHz, D_2O, δ): 3.40 (d, J = 5.9 Hz, 1H), 3.14 (s, 4H), 1.95 – 1.79 (m, 1H)), f) *N,N,N′,N′*-tetramethyl-1,6-diaminohexane (^{1}H NMR (300 MHz, D_2O,δ): 2.26 (dd, J = 17.1, 9.1 Hz, 4H), 2.15 (s, 12H), 1.56 – 1.36 (m, 4H), 1.29 (d, J = 6.7 Hz, 4H)) and HM6I (^{1}H NMR (300 MHz, D_2O, δ): 3.41 – 3.28 (m, 1H), 3.12 (s, 4H), 1.83 (d, J = 2.7 Hz, 1H), 1.54 – 1.36 (m, 1H)), g) *N,N,N′,N′*-tetramethyl-1,6-diaminohexane (^{13}C NMR (75 MHz, D_2O, δ): 58.68 (s), 43.93 (s), 26.74 (s), 26.33 (s)) and HM6I (^{13}C NMR (75 MHz, D_2O, δ): 66.52 (s), 53.39 – 52.86 (m), 25.09 (s), 22.29 (s)), h) 1,8-diaminooctane (^{1}H NMR (300 MHz, D_2O, δ): 2.65 (t, J = 7.0 Hz, 4H), 1.57 – 1.43 (m, 4H), 1.38 (s, 8H)) and HM8I (^{1}H NMR (300 MHz, D_2O, δ): 3.36 – 3.22 (m, 1H), 3.08 (s, 4H), 1.75 (d, J = 7.2 Hz, 1H), 1.36 (s, 2H)), i) 1,8-diaminooctane (^{13}C NMR (75 MHz, D_2O, δ): 40.91 (s), 32.39 (s), 29.13 (s), 26.57 (s)) and HM8I (^{13}C NMR (75 MHz, D_2O, δ): 66.78 (s), 53.25 – 52.77 (m), 27.92 (s), 25.31 (s), 22.32 (s), 16.59 (s)), and j) HE2I (^{1}H NMR (300 MHz, D_2O, δ): 3.70 (s, 1H), 3.45 (q, J = 7.2 Hz, 3H), 1.34 (t, J = 7.2 Hz, 4H)).

	Draw solute	Amine	Iodoalkane	Base
Monoammonium iodide salt	3MBAI	5	28	53
	3MOAI	5.0[a)]	22	11.6[a)]
	3PEAI	5	6	-
Diammonium iodide salt	HM2I	15	37	-
	HM4I	18	37	-
	HM6I	21	37	-
	HM8I	14.4[a)]	75	105
	HE2I	5	72	78

All units: mL (volume) except for [a)] g (weight).

Table S1. Amounts of reagents used for the synthesis of the ammonium iodide salts.

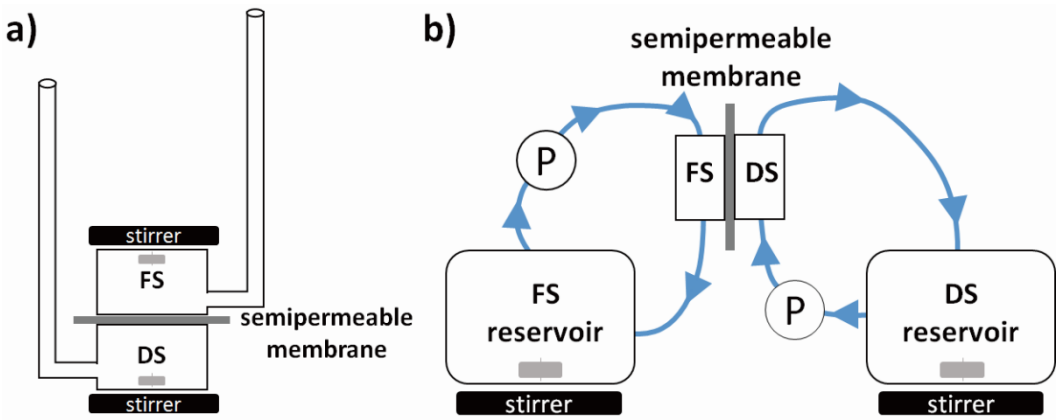


Figure S2. Schematic illustration of a) handmade U-shape glass tubes for small-scale analysis (dead-end type) and b) a cross-flow instrument for large-scale analysis.

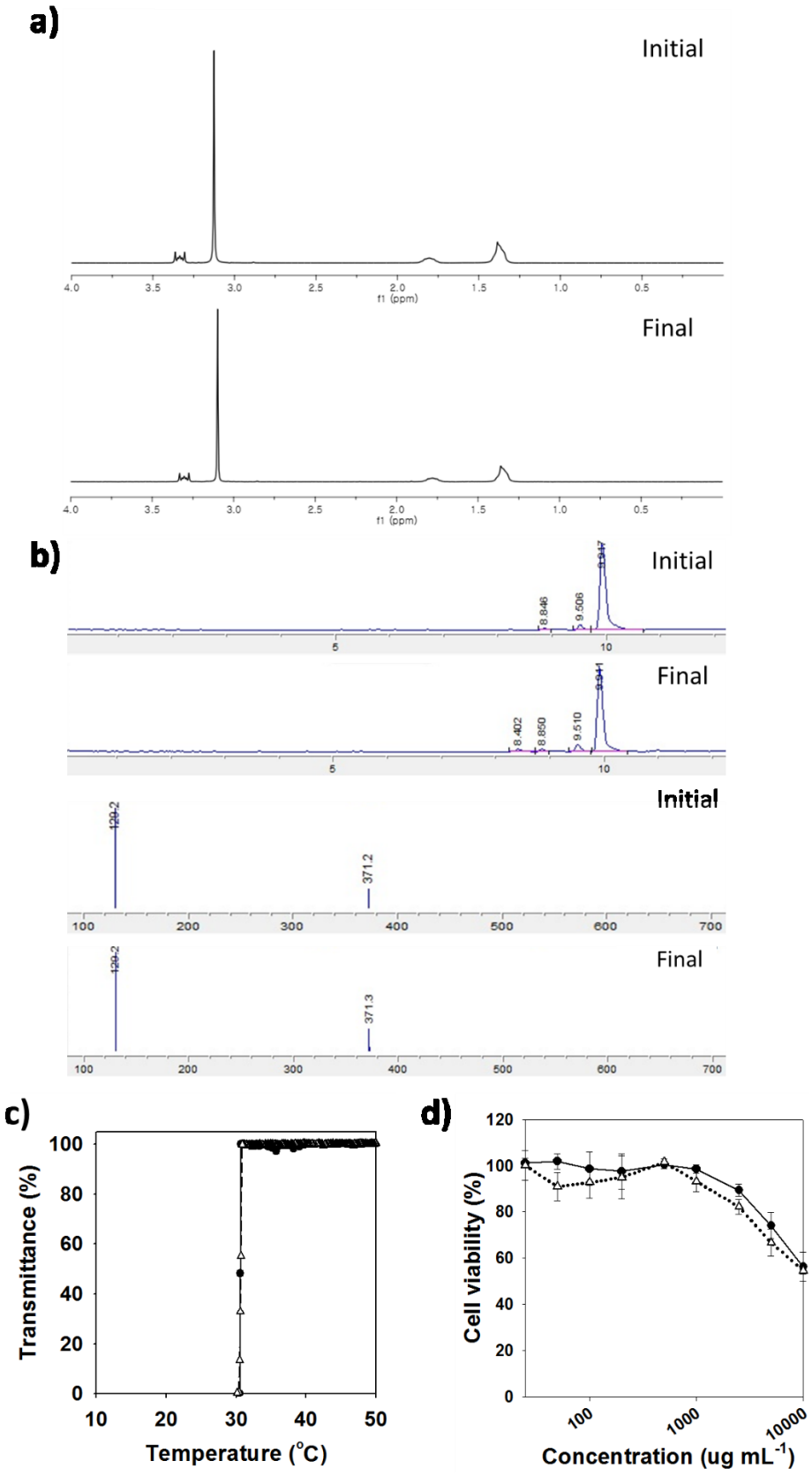


Figure S3. a) ^{1}H NMR spectra of HM10I before and after stability test. b) LC/MS spectra of HM10I before and after stability test. c) The UCST phase transition of aqueous solution of 40 wt% HM10I (initial (●, solid line) and after stability test (△, dash line)). d) Viability of HeLa cells treated with HM8I (●, solid line) and HM10I (△, dotted line). Each data point represents the average value of five experiments (±S.D.).