Supplementary Information

Structural optimization of super-gelators derived from naturally-occurring mannose and their morphological diversity

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1. General information

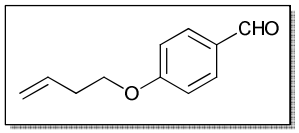
^{1}H NMR spectra are recorded either on JEOL JNM-ECA 600 (600 MHz for ^{1}H) spectrometer. Chemical shifts are reported in parts per million downfield (δ) relative to internal tetramethylsilane (TMS, δ_H 0.00). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz), intergration, and assignment. ^{13}C NMR spectra are recorded either on JEOL JNM-ECA 600 (150 MHz for ^{13}C) spectrometer with complete proton decoupling. Chemical shifts are reported in perts per million downfield (δ) relative to solvent as the internal standard ($CDCl_3$, δ_C 77.0). EI and FAB mass spectra were measured on JEOL JMS-700. TEM imaging was performed on a JEOL JEM-2010HCKM at the Reseach Laboratory for High Voltage Electron Microscopy, Kyushu University. FE-SEM imaging was performed on a Hitachi SU-8000 at the Center of Advanced Instrumental Analysis, Kyushu University. AFM was performed on

an SII NanoTechnology Inc. Nanonavi/Nanocute (now Hitachi High-Tech Science Corp.). Frash chromatography was performed on a Shoko Scientific Co., Ltd. Purif-espoir2 and Pulif-Pack SI-60. Merck precoated TLC plates (silica gel 60 F254) were used. Anhydrous DMF and MeOH were purchased from Wako Pure Chemical.

2. Synthesis

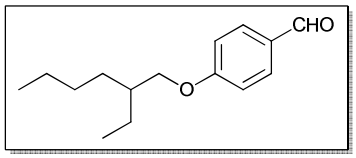
2-1. Synthesis of 4-alkoxybenzaldehydes

4-(3-butenyloxy)benzaldehyde [S1]



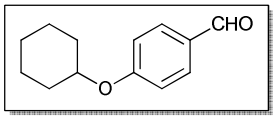
A mixture of 4-hydroxybenzaldehyde (4.9 g, 40 mmol), 4-bromo-1-butene (13.5 g, 100 mmol) and potassium carbonate (8.3 g, 60 mmol) in anhydrous DMF (80 mL) were stirred for 6 h at 80 °C. The reaction mixture cooled to rt and filtered. The filtrate was concentrated under reduced pressure. To the residue was added brine and extracted with ethyl acetate. The extract was washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2; the hexane/ethyl acetate ratio varying from 90/10, vol/vol) to give the desired product (5.9 g, 84%) as clear oil. δ_H (600 MHz, $CDCl_3$): 9.88 (1H, s), 7.85–7.81 (2H, m), 7.02–6.95 (2H, m), 5.95–5.86 (1H, m), 5.22–5.12 (2H, m), 4.15–4.05 (2H, m), 2.61–2.55 (2H, m).

4-(2-Ethylhexyloxy)benzaldehyde [S2]



A mixture of 4-hydroxybenzaldehyde (4.9 g, 40 mmol), 2-ethylhexylbromide (9.7 g, 50 mmol) and potassium carbonate (8.3 g, 60 mmol) in anhydrous DMF (80 mL) were stirred for 3 h at 80 °C. The reaction mixture cooled to rt and filtered. The filtrate was concentrated under reduced pressure. To the residue was added brine and extracted with ethyl acetate. The extract was washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2; the hexane/ethyl acetate ratio varying from 90/10, vol/vol) to give the desired product (8.9 g, 95%) as clear oil. δ_H (600 MHz, $CDCl_3$): 9.88 (1H, s), 7.85–7.81 (2H, m), 7.02–6.98 (2H, m), 3.94–3.91 (2H, m), 1.78–1.73 (1H, m), 1.53–1.30 (8H, m), 0.95–0.85 (6H, m).

4-cyclohexyloxybenzaldehyde



A mixture of 4-hydroxybenzaldehyde (10.0 g, 82 mmol), bromocyclohexane (15.0 mL, 122 mmol), tetrabutylammonmium

iodide (0.25 g, 0.67 mmol) and potassium carbonate (34.0 g, 246 mmol) in anhydrous DMF (80 mL) were stirred for 12 h at 150 °C. The reaction mixture cooled to rt and filtered. The filtrate was concentrated under reduced pressure. To the residue was added brine and extracted with ethyl acetate. The extract was washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2; the hexane/ethyl acetate ratio varying from 90/10, vol/vol) to give the desired product (2.0 g, 12%) as clear oil. δ_H (600 MHz, $CDCl_3$): 9.85 (1H, s), 7.83–7.79 (2H, m), 7.00–6.96 (2H, m), 4.41–4.35 (1H, m), 2.05–1.98 (2H, m), 1.87–1.79 (2H, m), 1.63–1.50 (3H, m), 1.45–1.29 (3H, m).

2-2. Synthesis of mannose derivatives

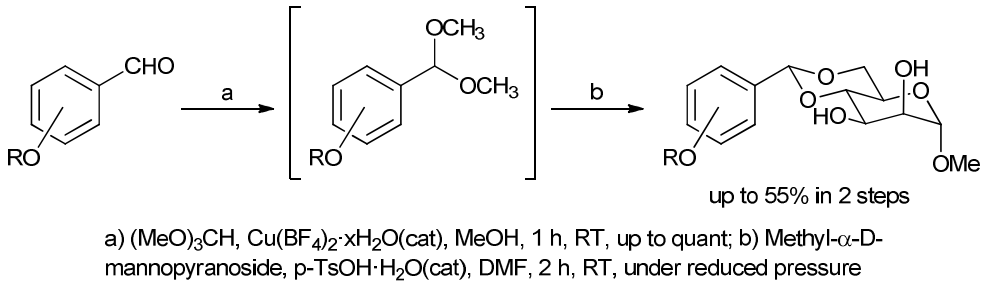
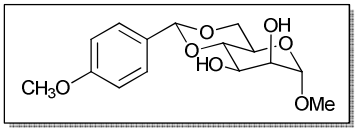


Figure S1. Synthesis scheme of mannose derivatives

General procedure: Copper(II) tetrafluoroborate (0.2 mmol) was added to a mixture of 4-alkoxybenzaldehyde (20 mmol) and trimethyl orthoformate (40 mmol) in anhydrous methanol (8 mL) under nitrogen atmosphere. The reaction mixture was stirred for 1 h at RT. After 1 h, the reaction mixture was quenched with saturated $NaHCO_3$ and extracted with ethyl acetate. The extracts were washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The obtained clear oil or pale yellow oil was used in the next reaction without further purification.

A solution of crude dimethylacetal in DMF (10 mL) was added dropwise to a suspension of methyl-α-D-mannopyranoside (22 mmol) and *p*-toluenesulfonic acid (0.5 mmol) in anhydrous DMF (20 mL) under nitrogen atmosphere. The reaction mixture was first stirred for 10 min at RT and then for 2 h under reduced pressure at RT. After 2 h, the reaction mixture was quenched with saturated $NaHCO_3$ and extracted with ethyl acetate. The extracts were washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography (SiO_2; the hexane/ethyl acetate ratio varying from 70/30 to 50/50, vol/vol). The desired product was then obtained.

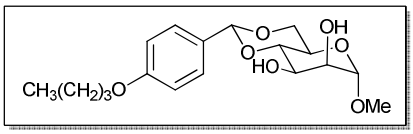
Methyl-4,6-*O*-(4-methoxybenzylidene)-α-D-mannopyranoside (1)



White solid, yield 55%

δ_H (600 MHz, $CDCl_3$): 7.39 (2H, d, J = 8.8 Hz), 6.88 (2H, d, J = 8.8 Hz), 5.52 (1H, s), 4.75 (1H, s), 4.30–4.22 (1H, m), 4.07–4.00 (2H, m), 3.93–3.86 (1H, m), 3.85–3.76 (5H, m), 3.40 (3H, s), 2.70–2.63 (2H, br). δ_C (150 MHz, $CDCl_3$): 160.26, 129.70, 127.57, 113.72, 102.21, 101.22, 78.82, 70.82, 68.81, 68.69, 62.87, 55.30, 55.09. HRMS (EI+): m/z calc'd for $C_{15}H_{20}O_7$ (M+): 312.1209; found: 312.1202.

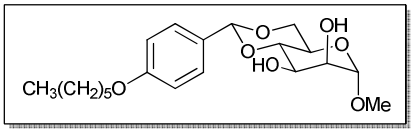
Methyl-4,6-*O*-(4-butoxybenzylidene)-α-D-mannopyranoside (2)



White solid, yield 45%

δ_H (600 MHz, $CDCl_3$): 7.40 (2H, d, J = 8.5 Hz), 6.89 (2H, d, J = 8.8 Hz), 5.52 (1H, s), 4.77 (1H, s), 4.31–4.22 (1H, m), 4.10–4.02 (2H, m), 3.96 (2H, t, J = 6.6 Hz), 3.93–3.86 (1H, m), 3.85–3.76 (2H, m), 3.40 (3H, s), 2.66–2.60 (2H, br), 1.80–1.71 (2H, m), 1.53–1.43 (2H, m), 0.97 (3H, t, J = 7.6 Hz). δ_C (150 MHz, $CDCl_3$): 159.86, 129.46, 127.51, 114.32, 102.29, 101.21, 78.81, 70.82, 68.82, 68.73, 67.75, 62.89, 55.10, 31.23, 19.20, 13.82. HRMS (EI+): m/z calc'd for $C_{18}H_{26}O_7$ (M+): 354.1679; found: 354.1682.

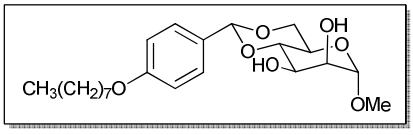
Methyl-4,6-*O*-(4-hexyloxybenzylidene)-α-D-mannopyranoside (3)



White solid, yield 49%

δ_H (600 MHz, $CDCl_3$): 7.39 (2H, d, J = 8.8 Hz), 6.88 (2H, d, J = 8.6 Hz), 5.52 (1H, s), 4.76 (1H, s), 4.30–4.22 (1H, m), 4.09–4.02 (2H, m), 3.95 (2H, t, J = 6.5 Hz), 3.92–3.86 (1H, m), 3.84–3.76 (2H, m), 3.40 (3H, s), 2.64–2.59 (2H, br), 1.80–1.73 (2H, m), 1.48–1.40 (2H, m), 1.38–1.29 (4H, m), 0.93–0.86 (3H, m). δ_C (150 MHz, $CDCl_3$): 159.86, 129.45, 127.51, 114.32, 102.29, 101.21, 78.81, 70.82, 68.82, 68.72, 68.08, 62.87, 55.10, 31.56, 29.16, 25.67, 22.59, 14.02. HRMS (EI+): m/z calc'd for $C_{20}H_{30}O_7$ (M+): 382.1992; found: 382.1997.

Methyl-4,6-*O*-(4-octyloxybenzylidene)-α-D-mannopyranoside (4)

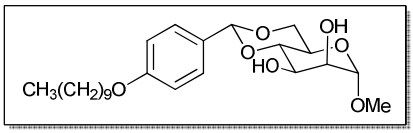


White solid, yield 48%

δ_H (600 MHz, $CDCl_3$): 7.39 (2H, d, J = 8.6 Hz), 6.88 (2H, d, J = 8.6 Hz), 5.52 (1H, s), 4.76 (1H, s), 4.30–4.23 (1H, m), 4.08–4.02 (2H, m), 3.95 (2H, t, J = 6.5 Hz), 3.92–3.86 (1H, m), 3.85–3.76 (2H, m), 3.40 (3H, s), 2.65–2.59 (2H, br), 1.80–1.73 (2H, m), 1.47–1.40 (2H, m), 1.37–1.22 (8H, m), 0.92–0.85 (3H, m). δ_C (150 MHz, $CDCl_3$): 159.86, 129.45, 127.51,

114.32, 102.29, 101.22, 78.81, 70.82, 68.82, 68.73, 68.09, 62.87, 55.10, 31.80, 29.34, 29.22, 29.19, 26.00, 22.64, 14.08. HRMS (EI+): m/z calc'd for $C_{22}H_{34}O_7$ (M+): 410.2305; found: 410.2308.

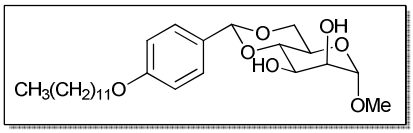
Methyl-4,6-*O*-(4-decyloxybenzylidene)-α-D-mannopyranoside (5)



White solid, yield 43%

δ_H (600 MHz, $CDCl_3$): 7.39 (2H, d, J = 8.8 Hz), 6.89 (2H, d, J = 8.8 Hz), 5.52 (1H, s), 4.76 (1H, s), 4.31–4.22 (1H, m), 4.09–4.01 (2H, m), 3.98–3.86 (3H, m), 3.85–3.76 (2H, m), 3.40 (3H, s), 2.66–2.60 (2H, m), 1.81–1.72 (2H, m), 1.48–1.38 (2H, m), 1.38–1.20 (12H, m), 0.88 (3H, d, J = 6.9 Hz). δ_C (150 MHz, $CDCl_3$): 159.86, 129.45, 127.51, 114.32, 102.29, 101.21, 78.81, 70.82, 68.82, 68.73, 68.09, 62.87, 55.10, 31.88, 29.56, 29.54, 29.38, 29.30, 29.19, 26.00, 22.66, 14.10. HRMS (EI+): m/z calc'd for $C_{24}H_{38}O_7$ (M+): 438.2618; found: 438.2615.

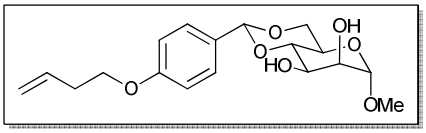
Methyl-4,6-*O*-(4-dodecyloxybenzylidene)-α-D-mannopyranoside (6)



White solid, yield 41%

δ_H (600 MHz, $CDCl_3$): 7.39 (2H, d, J = 8.8 Hz), 6.88 (2H, d, J = 8.5 Hz), 5.52 (1H, s), 4.76 (1H, s), 4.30–4.21 (1H, m), 4.08–4.01 (2H, m), 3.95 (2H, t, J = 6.6 Hz), 3.92–3.85 (1H, m), 3.84–3.75 (2H, m), 3.40 (3H, s), 2.69–2.62 (2H, m), 1.81–1.72 (2H, m), 1.48–1.39 (2H, m), 1.38–1.20 (16H, m), 0.88 (3H, d, J = 6.9 Hz). δ_C (150 MHz, $CDCl_3$): 159.85, 129.44, 127.51, 114.31, 102.28, 101.21, 78.81, 70.82, 68.81, 68.70, 68.08, 62.87, 55.08, 31.90, 29.63, 29.61, 29.58, 29.56, 29.37, 29.33, 29.18, 25.99, 22.67, 14.09. HRMS (EI+): m/z calc'd for $C_{26}H_{42}O_7$ (M+): 466.2931; found: 466.2923.

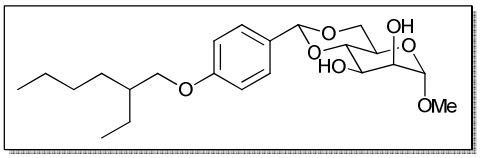
Methyl-4,6-*O*-(4-(3-butenyl)oxybenzylidene)-α-D-mannopyranoside (7)



White solid, yield 45%

δ_H (600 MHz, $CDCl_3$): 7.40 (2H, d, J = 8.8 Hz), 6.89 (2H, d, J = 8.5 Hz), 5.94–5.84 (1H, m), 5.52 (1H, s), 5.20–5.13 (1H, m), 5.13–5.08 (1H, m), 4.76 (1H, s), 4.31–4.22 (1H, m), 4.08–3.98 (4H, m), 3.93–3.86 (1H, m), 3.85–3.76 (2H, m), 3.40 (3H, s), 2.68–2.62 (2H, m), 2.57–2.50 (2H, m). δ_C (150 MHz, $CDCl_3$): 159.57, 134.29, 129.68, 127.56, 117.06, 114.37, 102.21, 101.23, 78.81, 70.82, 68.79, 68.64, 67.24, 62.88, 55.06, 33.53. HRMS (EI+): m/z calc'd for $C_{18}H_{24}O_7$ (M+): 352.1522; found: 352.1524.

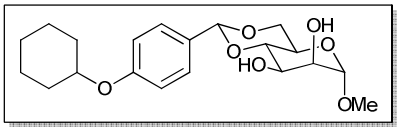
Methyl-4,6-O-(4-(2-ethylhexyl)oxybenzylidene)-α-D-mannopyranoside (8)



White solid, yield 40%

δ_H (600 MHz, $CDCl_3$): 7.39 (2H, d, J = 8.8 Hz), 6.88 (2H, d, J = 8.5 Hz), 5.50 (1H, s), 4.70 (1H, s), 4.28–4.20 (1H, m), 4.04–3.94 (2H, m), 3.91–3.73 (5H, m), 3.38 (3H, s), 2.98–2.83 (2H, m), 1.74–1.66 (1H, m), 1.54–1.24 (8H, m), 0.95–0.84 (6H, m). δ_C (150 MHz, $CDCl_3$): 160.04, 129.42, 127.50, 114.26, 102.18, 101.38, 78.73, 70.79, 70.58, 68.71, 68.50, 63.04, 54.89, 39.28, 30.45, 29.00, 23.80, 22.95, 13.97, 11.00. HRMS (EI+): m/z calc'd for $C_{22}H_{34}O_7$ (M+): 410.2305; found: 410.2304.

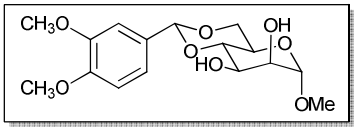
Methyl-4,6-*O*-(4-cyclohexyloxybenzylidene)-α-D-mannopyranoside (9)



White solid, yield 31%

δ_H (600 MHz, $CDCl_3$): 7.38 (2H, d, J = 8.6 Hz), 6.89 (2H, d, J = 8.8 Hz), 5.50 (1H, s), 4.74 (1H, d, J = 1.2 Hz), 4.28–4.21 (2H, m), 4.06–3.99 (2H, m), 3.91–3.85 (1H, m), 3.83–3.75 (2H, m), 3.39 (3H, s), 2.76 (1H, d, J = 3.4 Hz), 2.73 (1H, d, J = 2.2 Hz), 2.00–1.92 (2H, m), 1.82–1.74 (2H, m), 1.60–1.46 (3H, m), 1.40–1.25 (3H, m). δ_C (150 MHz, $CDCl_3$): 158.50, 129.38, 127.52, 115.80, 102.29, 101.22, 78.80, 75.35, 70.81, 68.79, 68.65, 62.88, 55.07, 31.65, 25.57, 23.66. HRMS (EI+): m/z calc'd for $C_{20}H_{28}O_7$ (M+): 380.1835; found: 380.1832.

Methyl-4,6-*O*-(3,4-dimethoxybenzylidene)-α-D-mannopyranoside (10)



White solid, yield 32%

δ_H (600 MHz, $CDCl_3$): 7.06–7.01 (2H, m), 6.86 (1H, d, J = 8.8 Hz), 5.53 (1H, s), 4.77 (1H, s), 4.32–4.24 (1H, m), 4.11–4.03 (2H, m), 3.94–3.78 (9H, m), 3.41 (3H, s), 2.72–2.64 (2H, br). δ_C (150 MHz, $CDCl_3$): 149.74, 148.95, 129.92, 119.02, 110.71, 109.10, 102.34, 101.24, 78.91, 70.84, 68.81, 68.62, 62.85, 55.93, 55.87, 55.09. HRMS (EI+): m/z calc'd for $C_{16}H_{22}O_8$ (M+): 342.1315; found: 342.1317.

References

S1 L. Tauk, A-P. Schroder, G. Decher and N. Giuseppone, *Nature Chem.*, 2009, **1**, 649–656.

S2 X. Chen, C-Y. Liu, T-H. Jeu, S-A. Chen and S. Holdcroft, *Chem. Mater.*, 2007, **19**, 5194–5199.

3. Pictures of gelation test

Figure S3-1. Gels of octane (0.1), cyclohexane (0.25), squalane (0.05), squalene (0.1), toluene (0.5), SH245 (0.05), olive oil (0.5) and IPM (0.5) formed from **1**. (Numbers in parentheses are CGC values (wt%).)

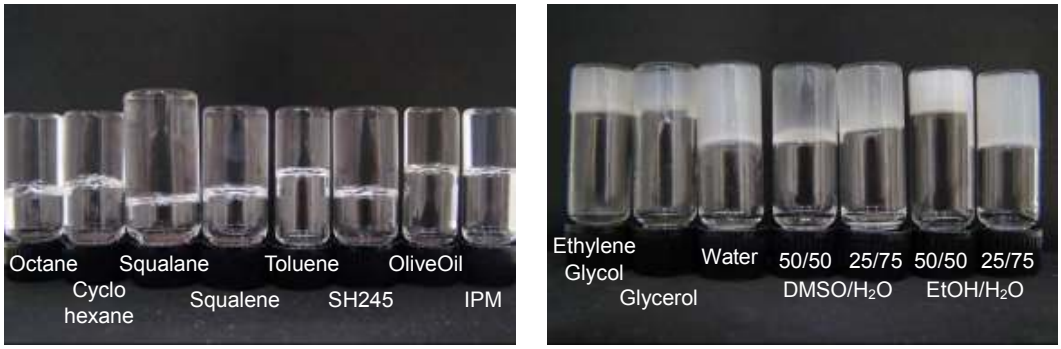


Figure S3-2. Gels of octane (0.05), cyclohexane (0.05), squalane (0.025), squalene (0.05), toluene (0.5), SH245 (0.05), olive oil (0.5), IPM (0.5), ethylene glycol (2.0), glycerol (2.0), water (0.1), DMSO/H_2O (50/50, vol/vol)) (0.5), DMSO/H_2O (25/75, vol/vol) (0.1), EtOH/H_2O (50/50, vol/vol)) (1.0) and EtOH/H_2O (25/75, vol/vol)) (0.1) formed from **2**. (Numbers in parentheses are CGC values (wt%).)

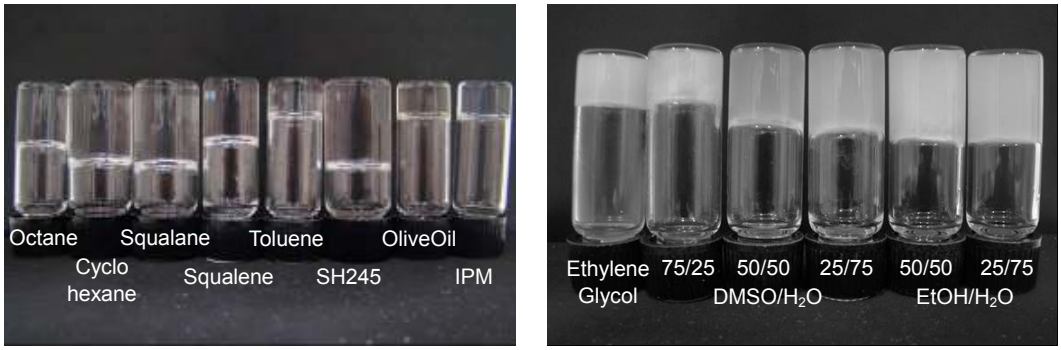


Figure S3-3. Gels of octane (0.1), cyclohexane (0.05), squalane (0.05), squalene (0.1), toluene (1.0), SH245 (0.05), olive oil (1.0), IPM (1.0), ethylene glycol (2.0), DMSO/H_2O (75/25, vol/vol)) (2.0), DMSO/H_2O (50/50, vol/vol)) (0.1), DMSO/H_2O (25/75, vol/vol) (0.1), EtOH/H_2O (50/50, vol/vol)) (0.5) and EtOH/H_2O (25/75, vol/vol)) (0.1) formed from **3**. (Numbers in parentheses are CGC values (wt%).)

Figure S3-4. Gels of octane (0.1), cyclohexane (0.1), squalane (0.05), squalene (0.25), toluene (1.0), SH245 (0.1), olive oil (1.0), IPM (1.0), ethylene glycol (1.0), DMSO/H_2O (75/25, vol/vol)) (1.0), DMSO/H_2O (50/50, vol/vol)) (0.05), DMSO/H_2O (25/75, vol/vol) (0.25), EtOH/H_2O (50/50, vol/vol)) (0.5) and EtOH/H_2O (25/75, vol/vol)) (0.05) formed from **4**. (Numbers in parentheses are CGC values (wt%).)

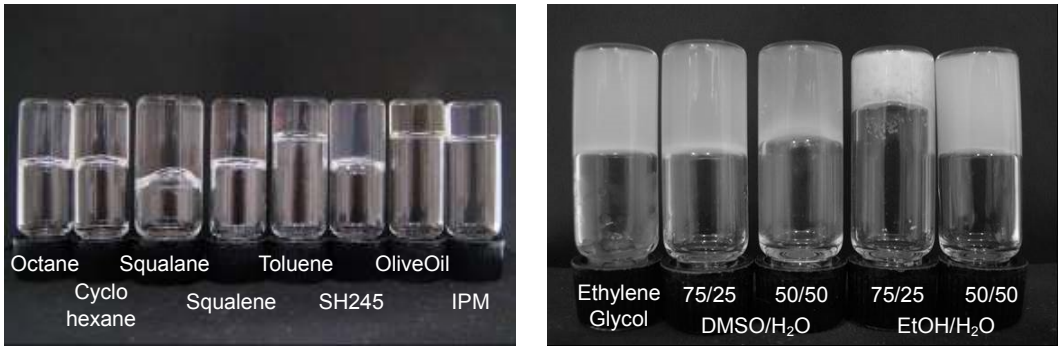


Figure S3-5. Gels of octane (0.1), cyclohexane (0.1), squalane (0.05), squalene (0.25), toluene (2.0), SH245 (0.25), olive oil (1.0), IPM (1.0), ethylene glycol (0.5), DMSO/H_2O (75/25, vol/vol)) (0.5), DMSO/H_2O (50/50, vol/vol)) (0.1), EtOH/H_2O (75/25, vol/vol)) (2.0) and EtOH/H_2O (50/50, vol/vol)) (0.25) formed from **5**. (Numbers in parentheses are CGC values (wt%).)

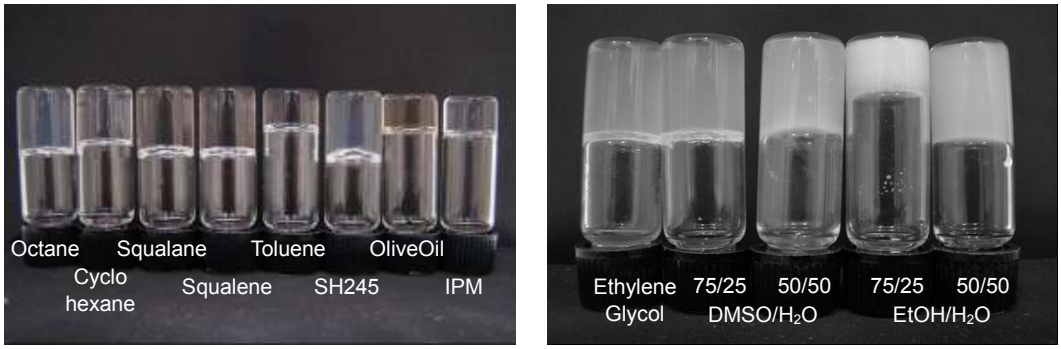
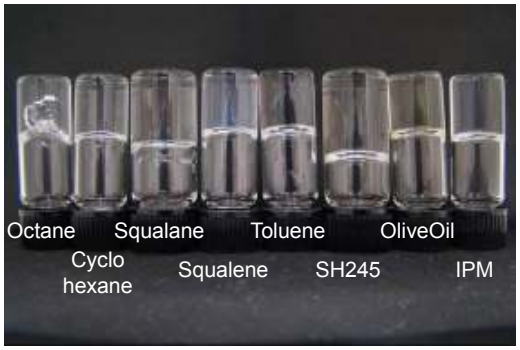


Figure S3-6. Gels of octane (0.25), cyclohexane (0.1), squalane (0.1), squalene (0.25), toluene (2.0), SH245 (0.5), olive oil (1.0), IPM (1.0), ethylene glycol (0.25), DMSO/H_2O (75/25, vol/vol)) (0.5), DMSO/H_2O (50/50, vol/vol)) (0.25), EtOH/H_2O (75/25, vol/vol)) (2.0) and EtOH/H_2O (50/50, vol/vol)) (0.25) formed from **6**. (Numbers in parentheses are CGC values (wt%).)



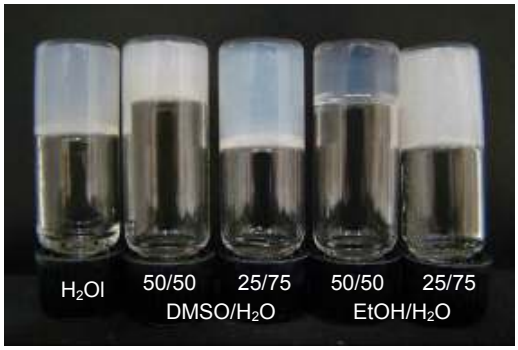


Figure S3-7. Gels of octane (0.1), cyclohexane (0.1), squalane (0.05), squalene (0.1), toluene (0.5), SH245 (0.05), olive oil (0.5), IPM (0.5), water (0.1), DMSO/H_2O (50/50, vol/vol)) (1.0), DMSO/H_2O (25/75, vol/vol)) (0.25), EtOH/H_2O (50/50, vol/vol)) (2.0) and EtOH/H_2O (25/75, vol/vol)) (0.25) formed from **7**. (Numbers in parentheses are CGC values (wt%).)

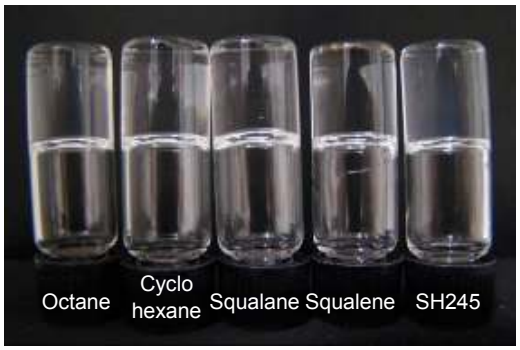


Figure S3-8. Gels of octane (0.05), cyclohexane (0.25), squalane (0.1), squalene (0.25) and SH245 (0.1) formed from **8**. (Numbers in parentheses are CGC values (wt%).)

4. FE-SEM and TEM images of xerogels

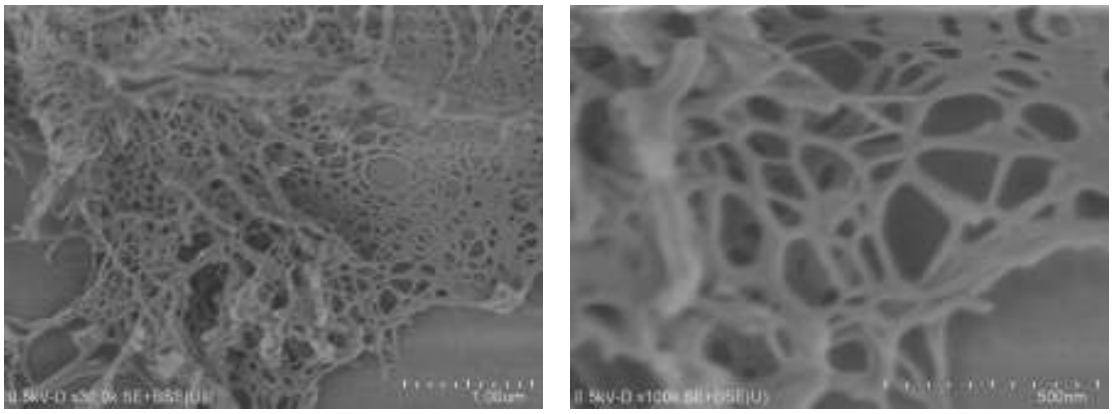


Figure S4-1. FE-SEM images of xerogel prepared from the cyclohexane gel of **2**.

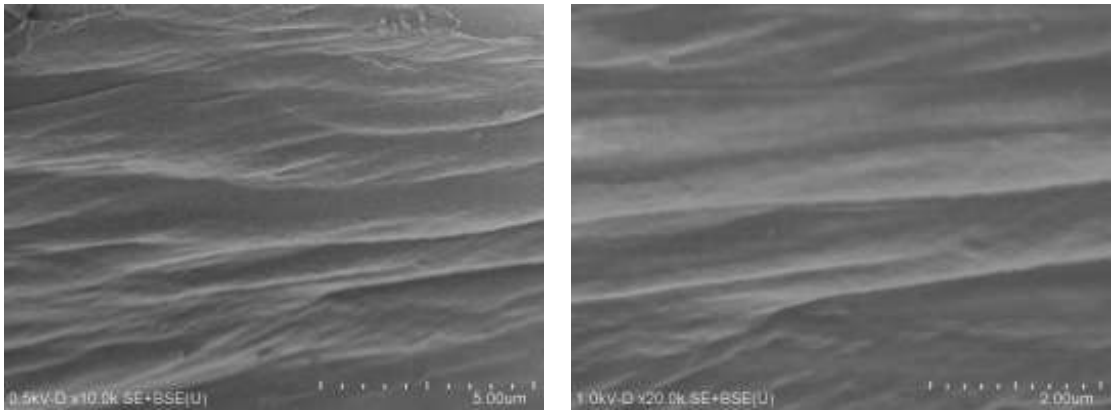


Figure S4-2. FE-SEM images of xerogel prepared from the toluene gel of **2**.

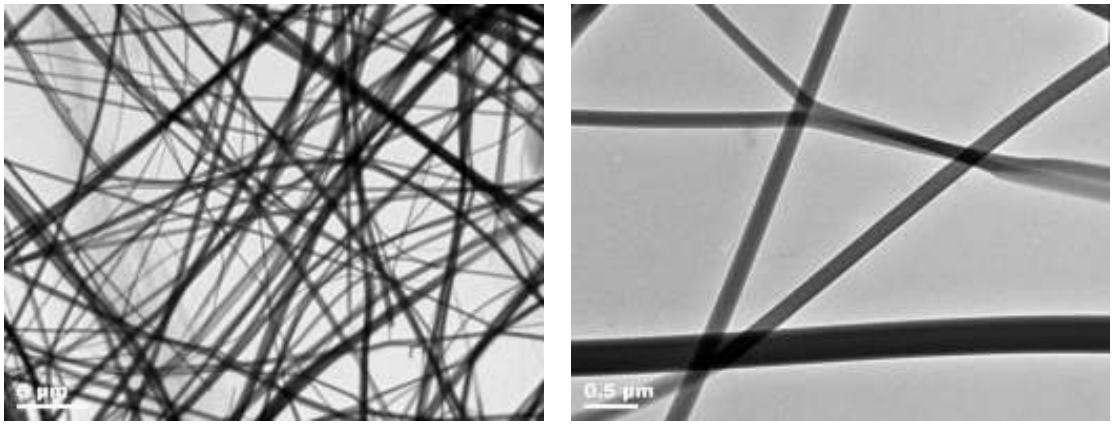


Figure S4-3. TEM images of the dried sample prepared from the toluene gel of **2**.

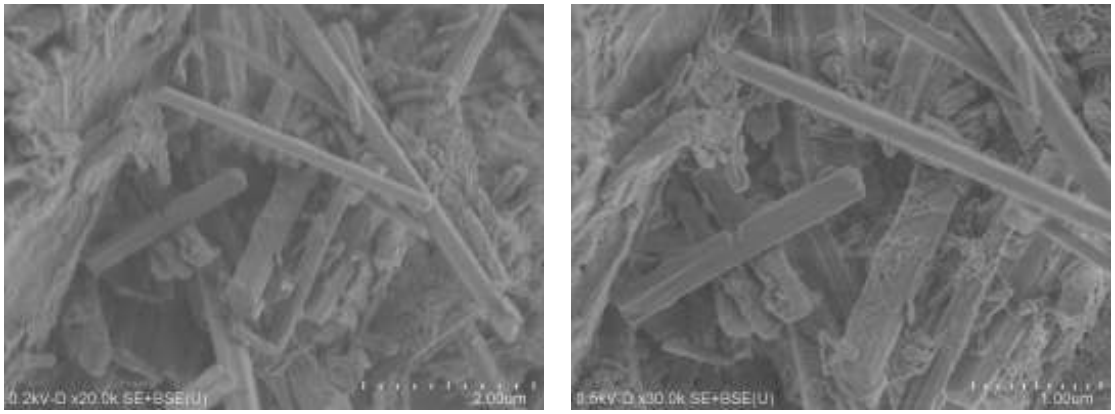


Figure S4-4. FE-SEM images of xerogel prepared from the EtOH/H_2O (50/50, vol/vol) gel of **2**.

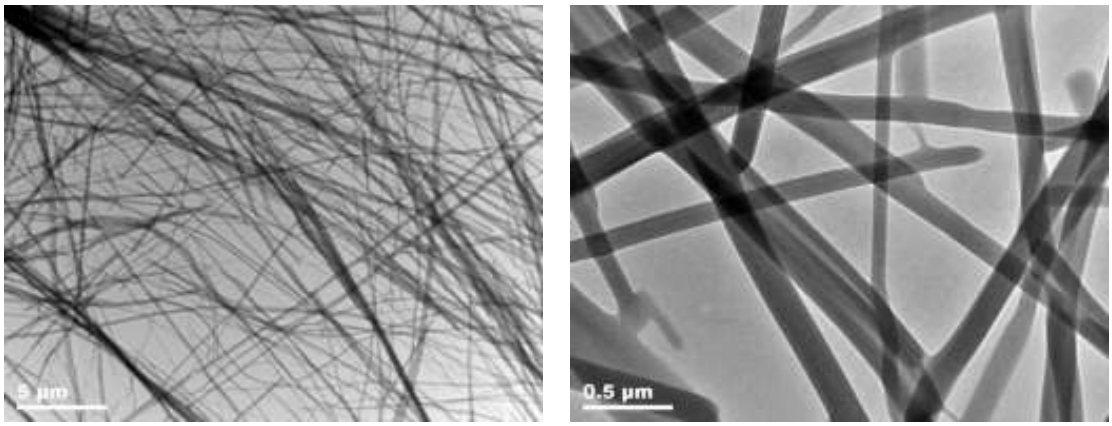


Figure S4-5. TEM images of the dried sample prepared from the EtOH/H_2O (50/50, vol/vol) gel of **2**.

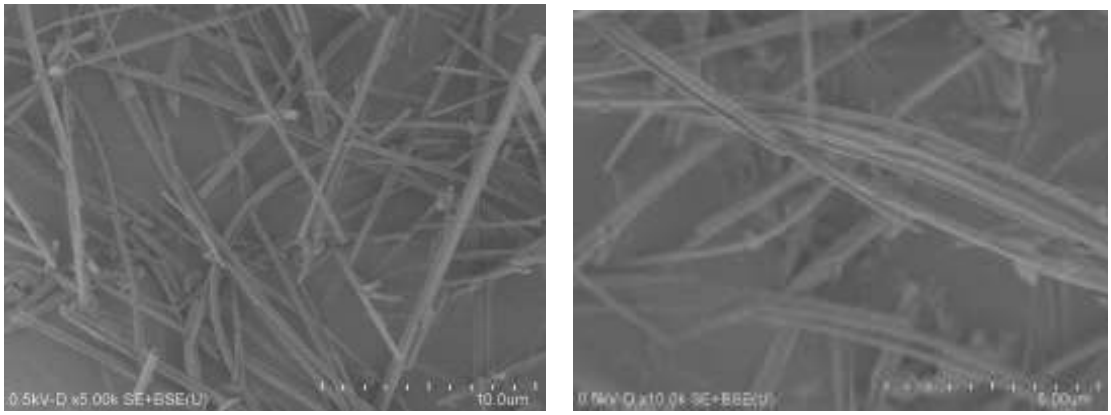


Figure S4-6. FE-SEM images of xerogel prepared from the hydrogel of **2**.

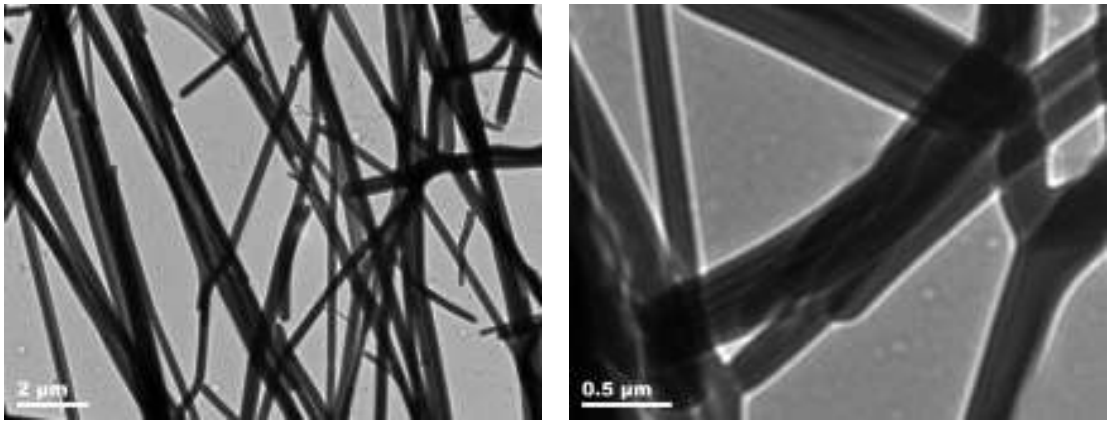


Figure S4-7. TEM images of the dried sample prepared from hydrogel of **2**.

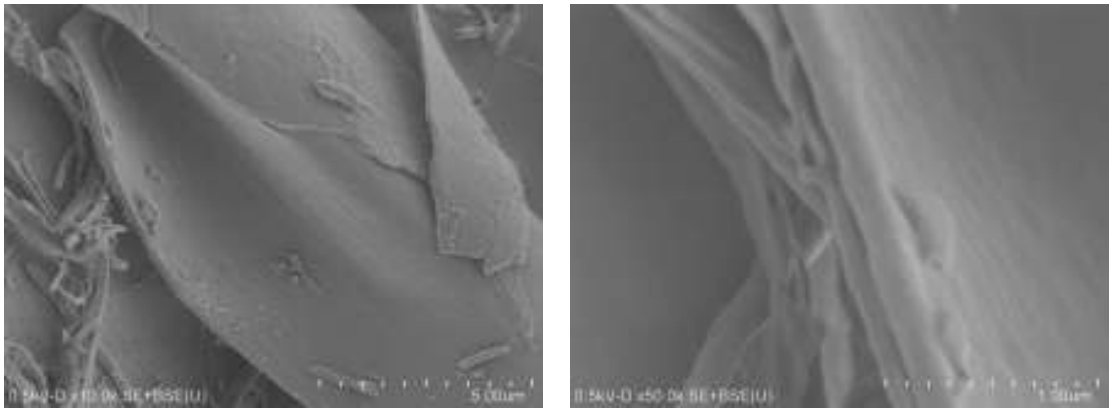


Figure S4-8. FE-SEM images of xerogel prepared from the cyclohexane gel of **6**.

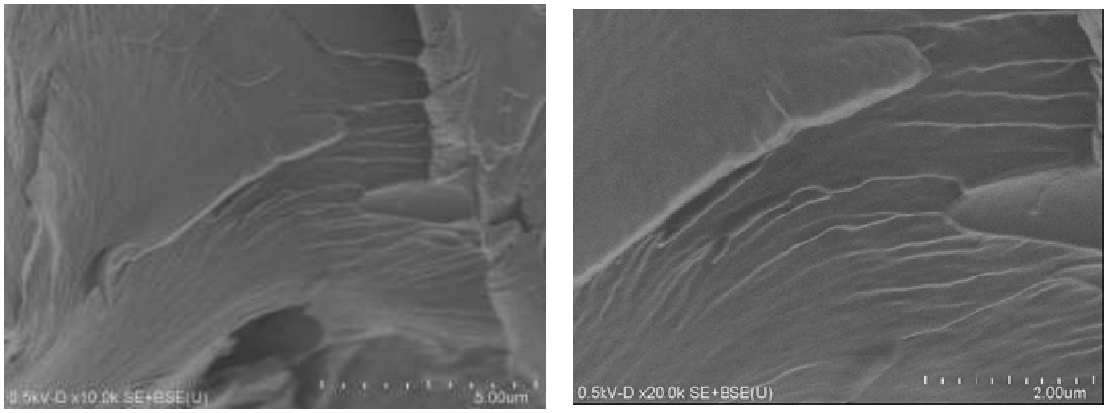


Figure S4-9. FE-SEM images of xerogel prepared from the toluene gel of **6**.

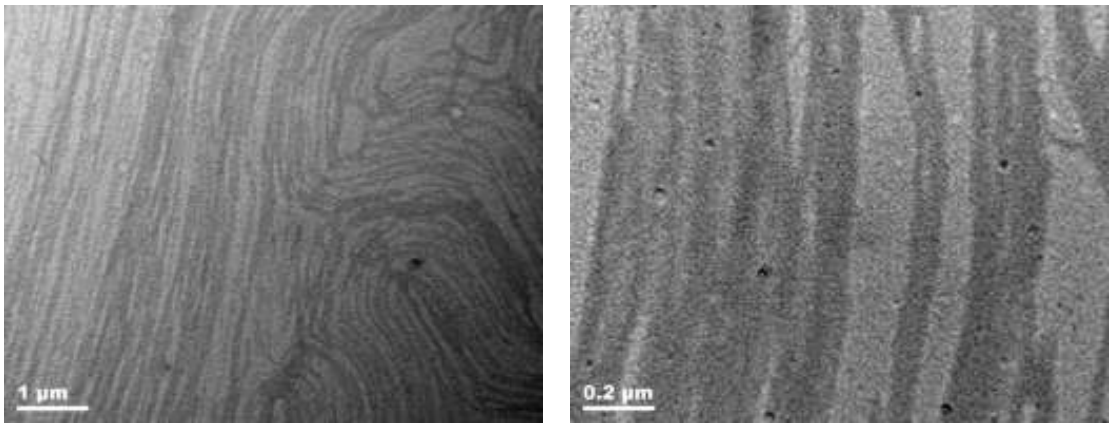


Figure S4-10. TEM images of the dried sample prepared from toluene gel of **6**.

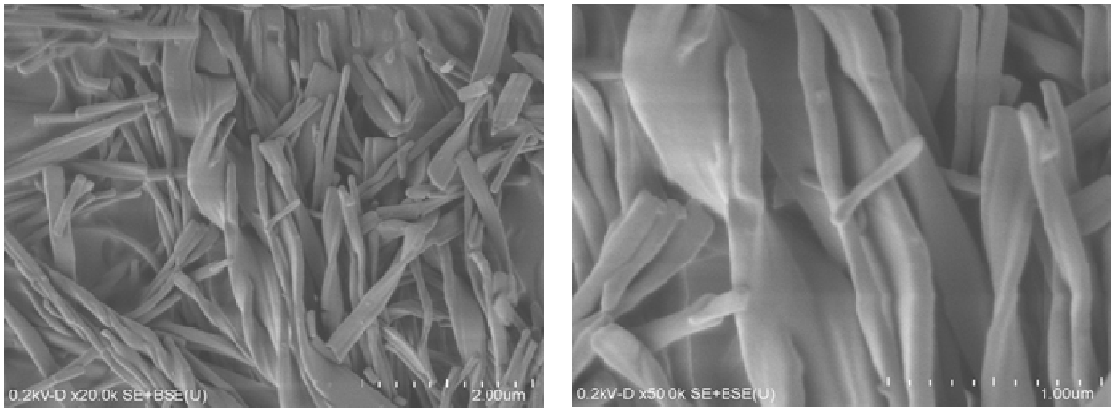


Figure S4-11. FE-SEM images of xerogel prepared from the EtOH/H_2O (50/50, vol/vol) gel of **6**.

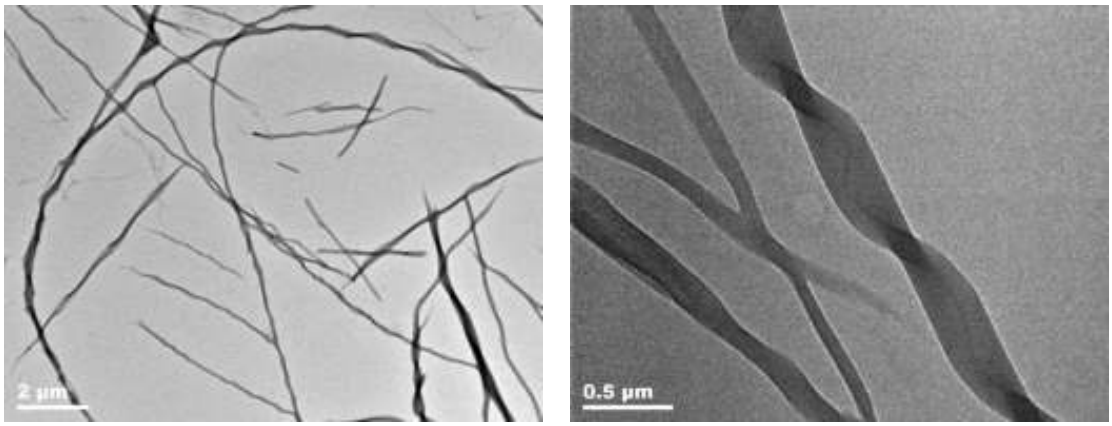


Figure S4-12. TEM images of the dried sample prepared from the EtOH/H_2O (50/50, vol/vol) gel of **6**.

5. AFM images of dried toluene solution for 2 and 6 at 0.02 wt%

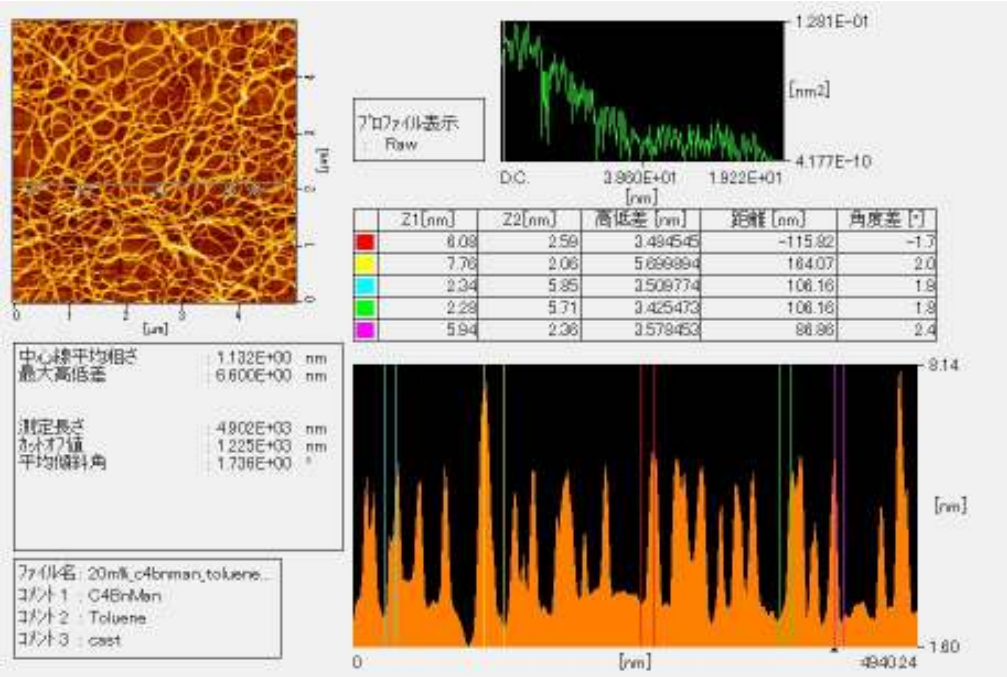


Figure S5-1. AFM image and the slice image of dried toluene solution of **2** at 0.02 wt% on HOPG.

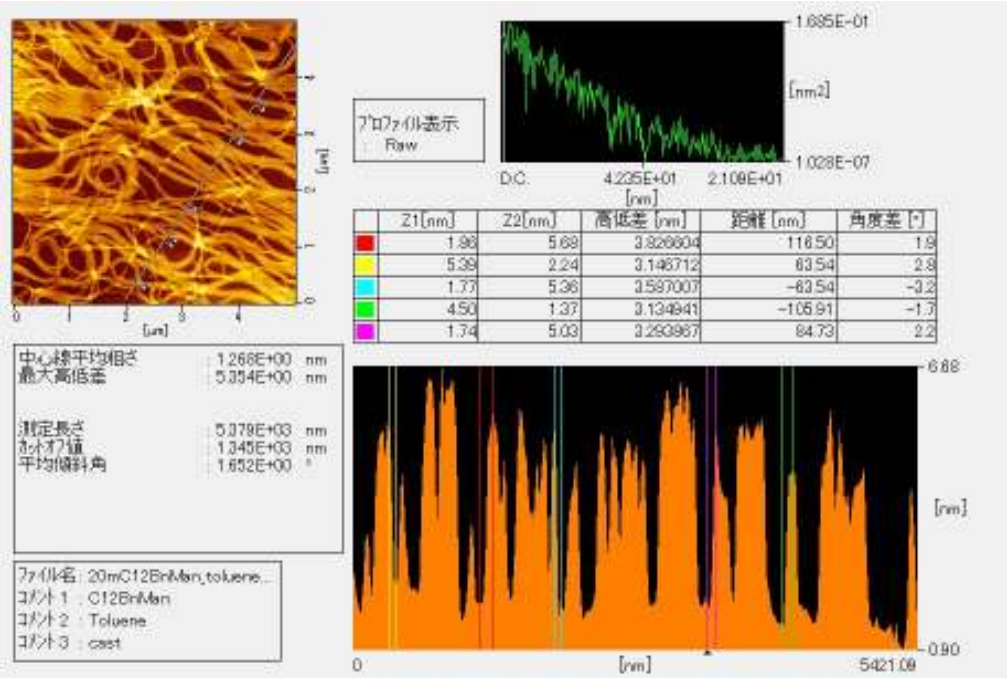
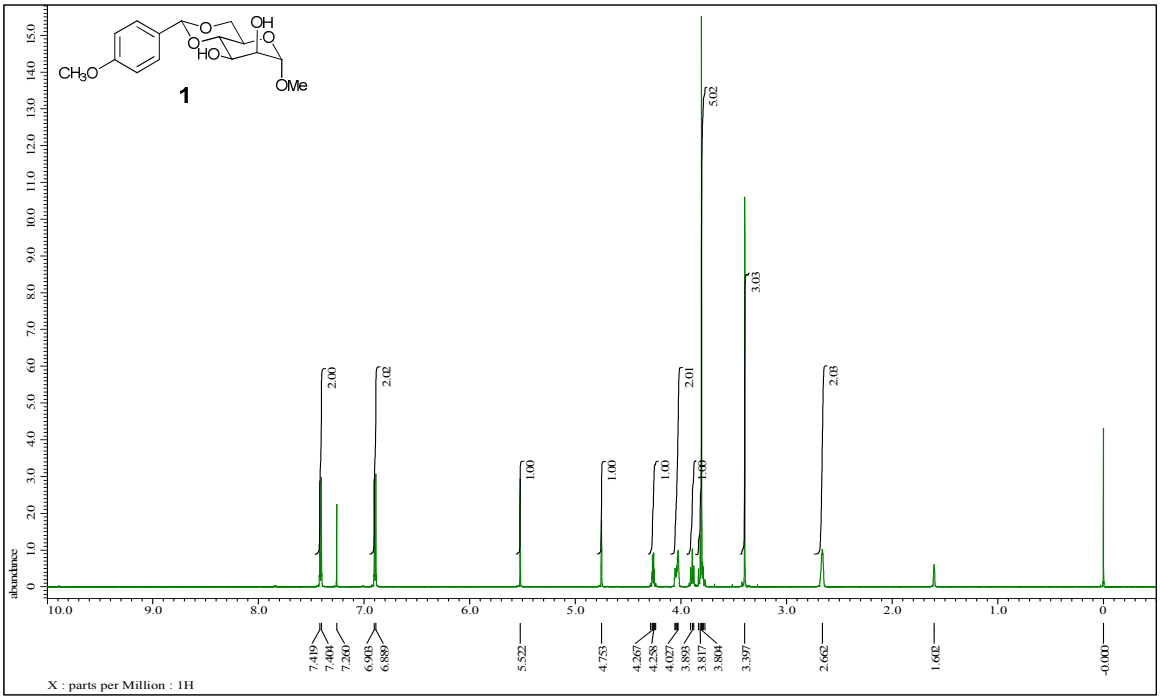
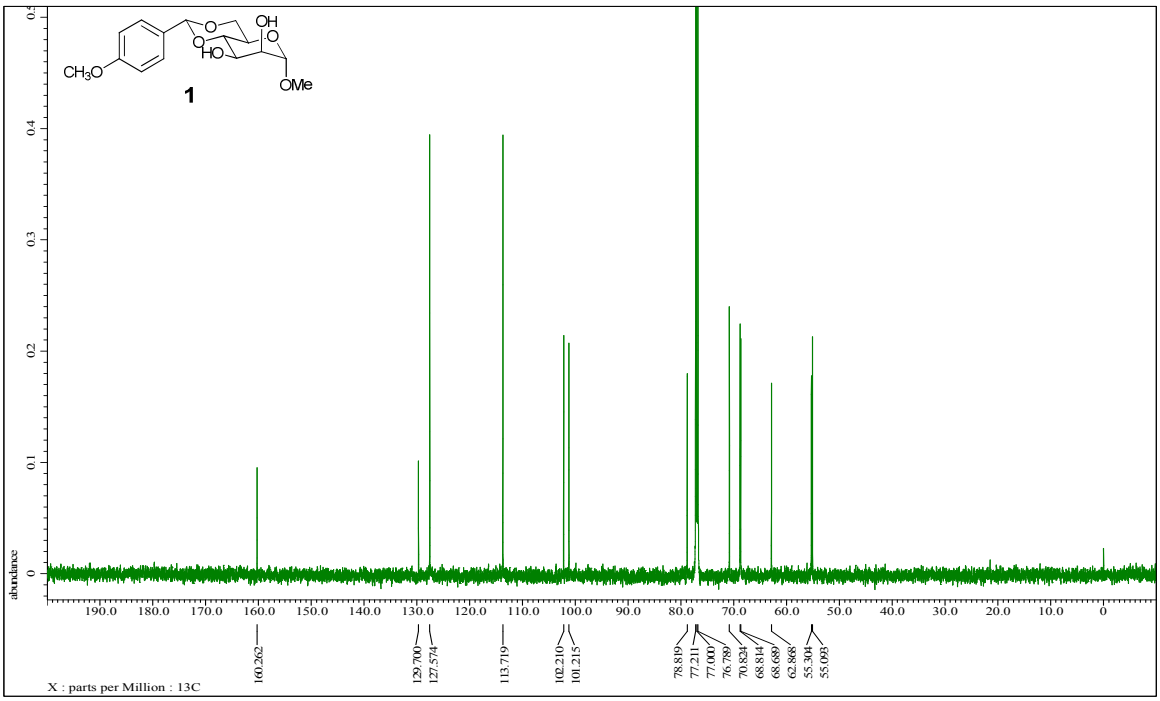
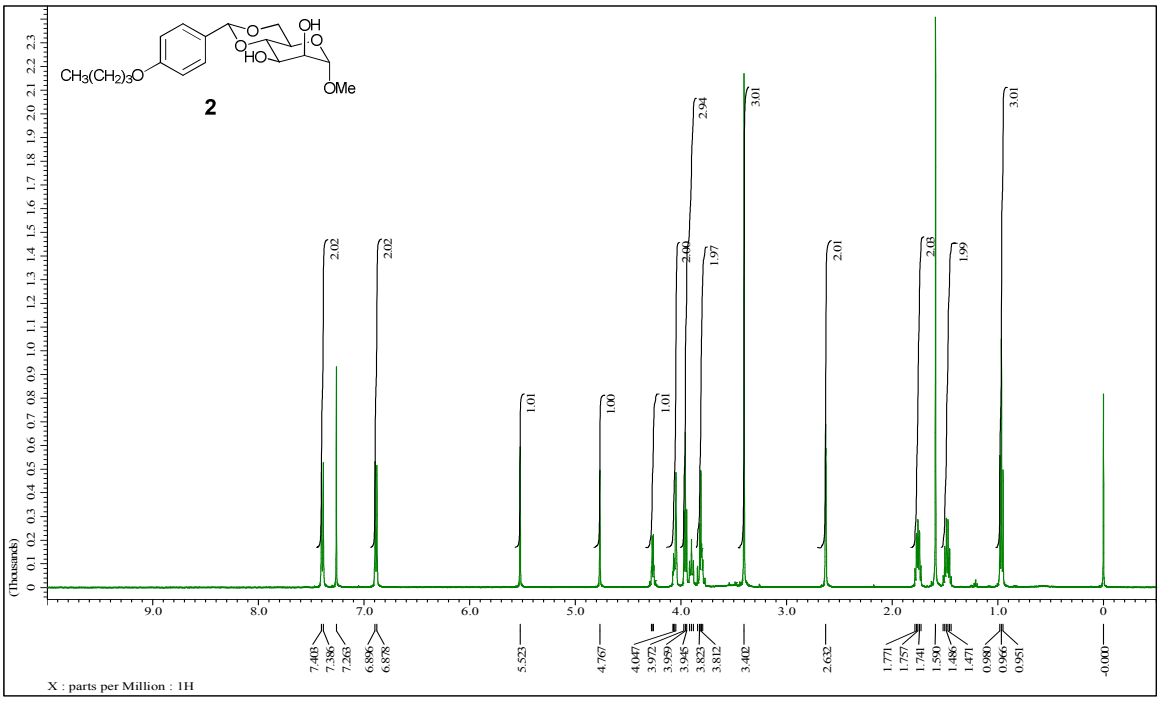


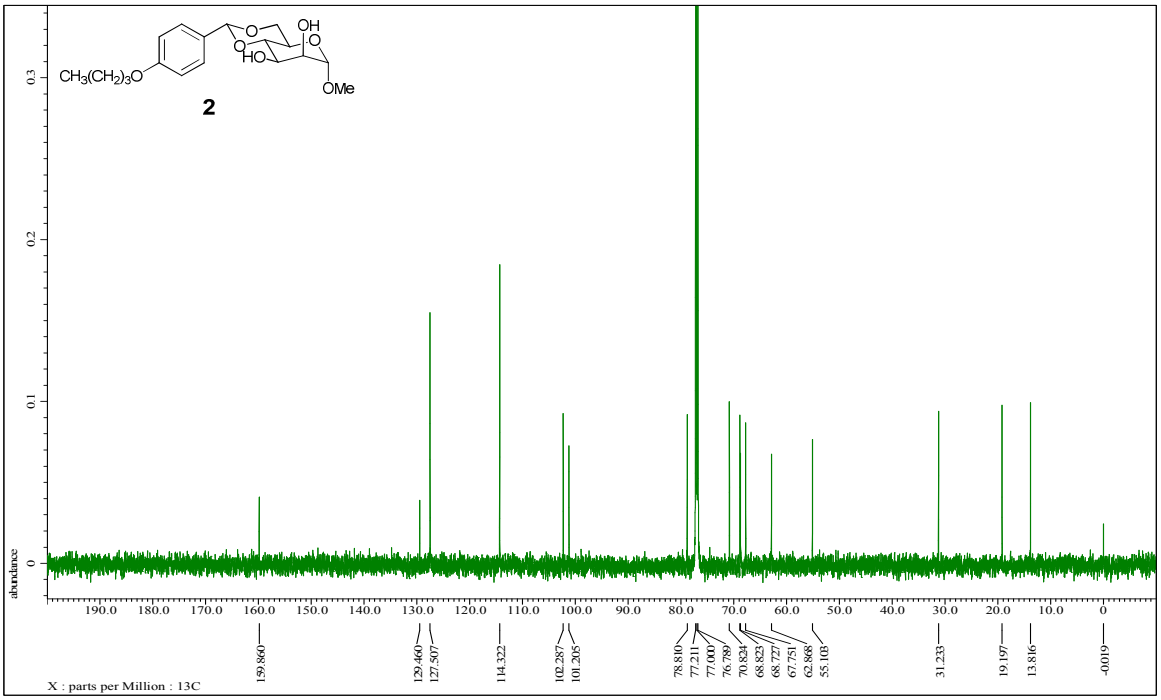
Figure S5-2. AFM image and the slice image of dried toluene solution of **6** at 0.02 wt% on HOPG.

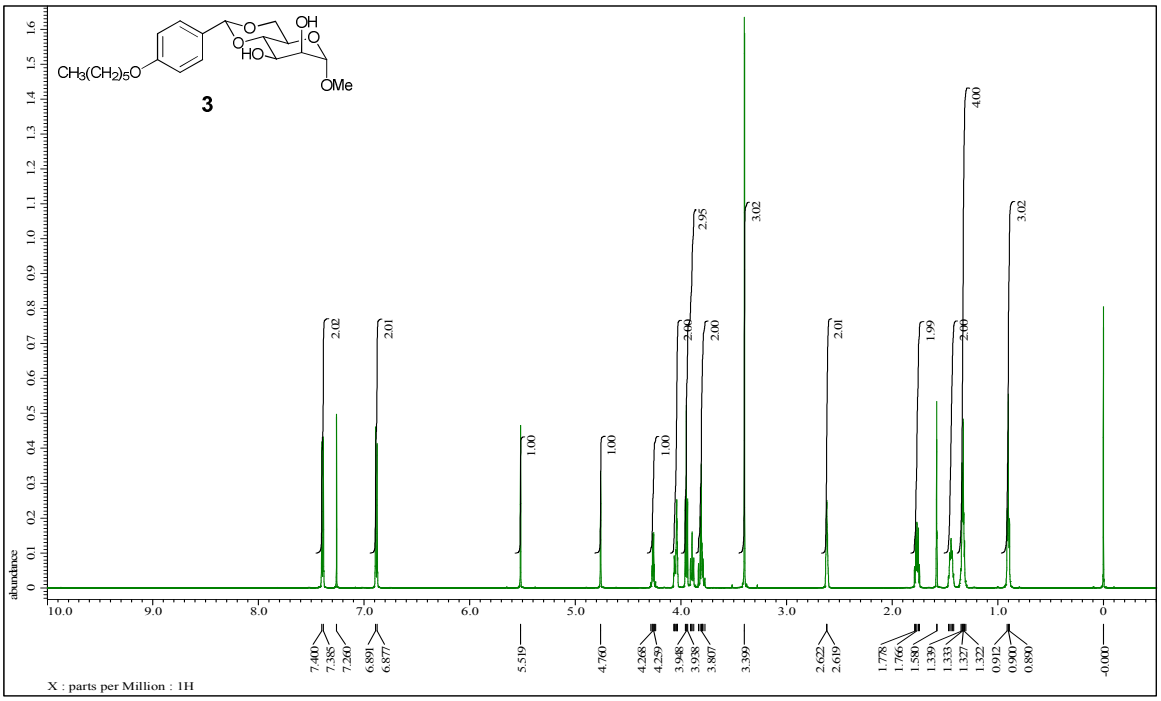
6. ^{1}H and ^{13}C NMR spectra of mannose derivatives

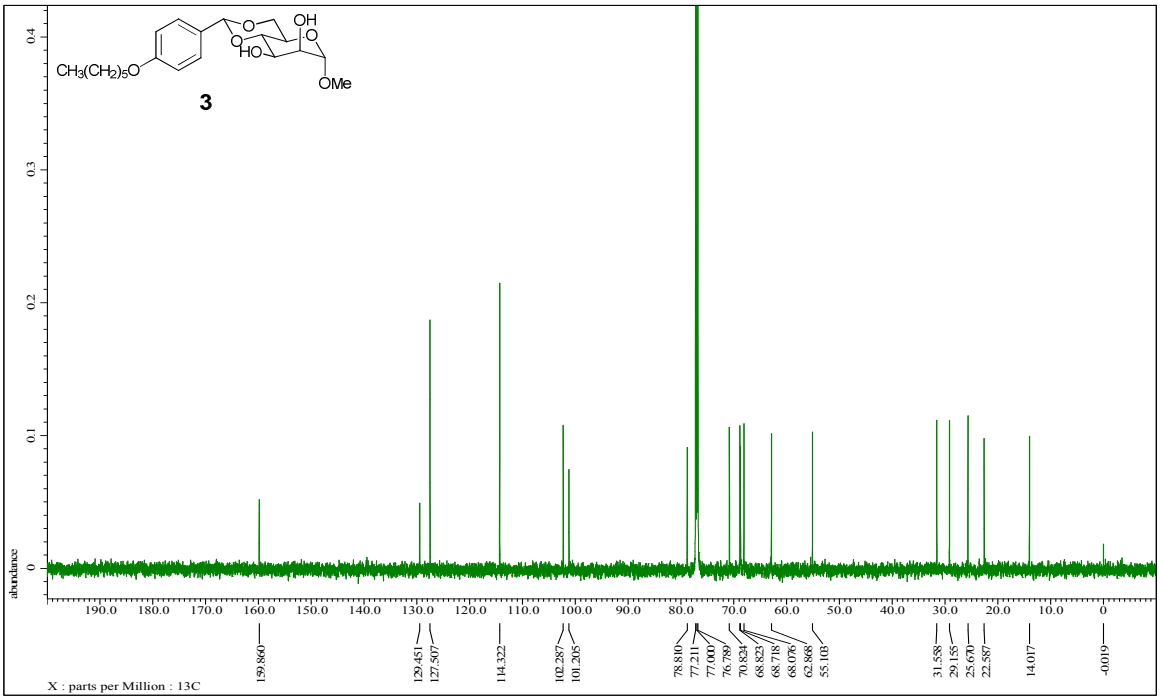


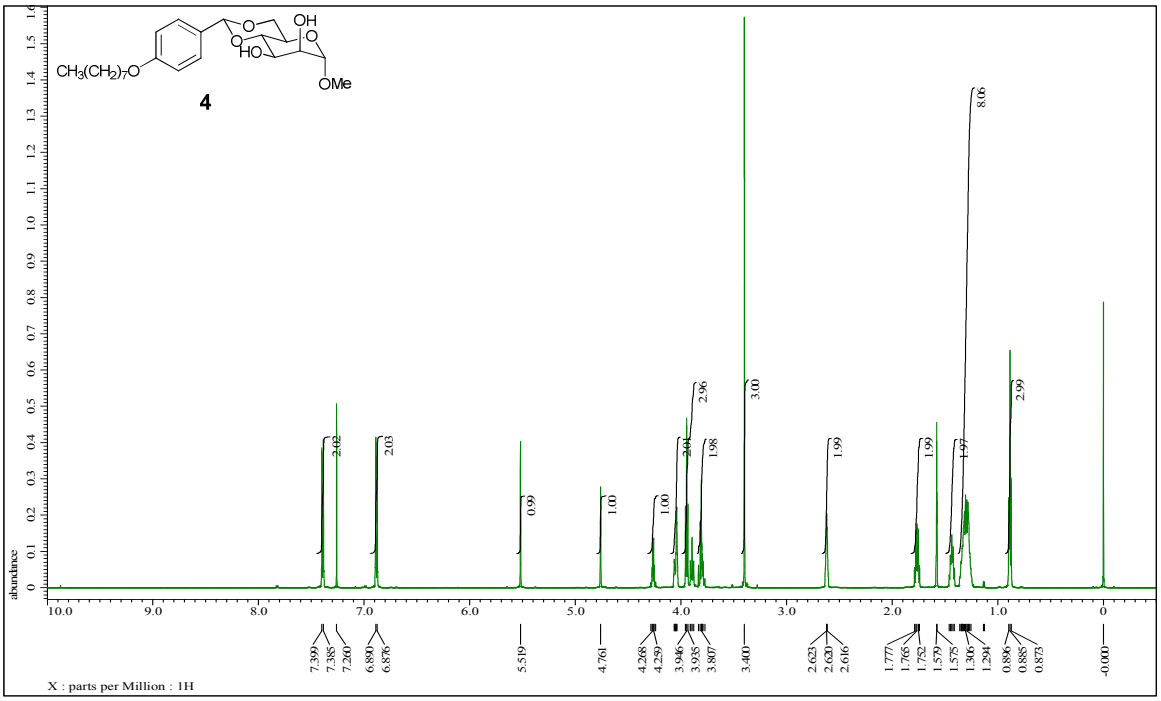


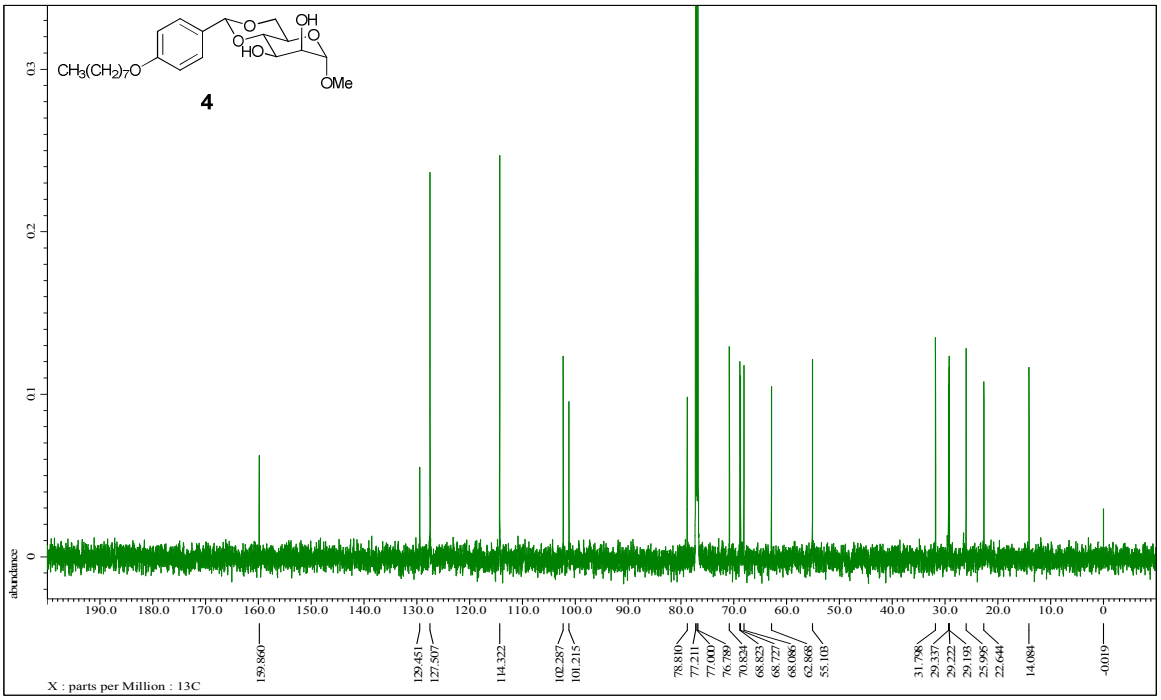

CH3(CH2)3O
OH
O
HO
OMe
2
(Thousands)
X : parts per Million : 1H

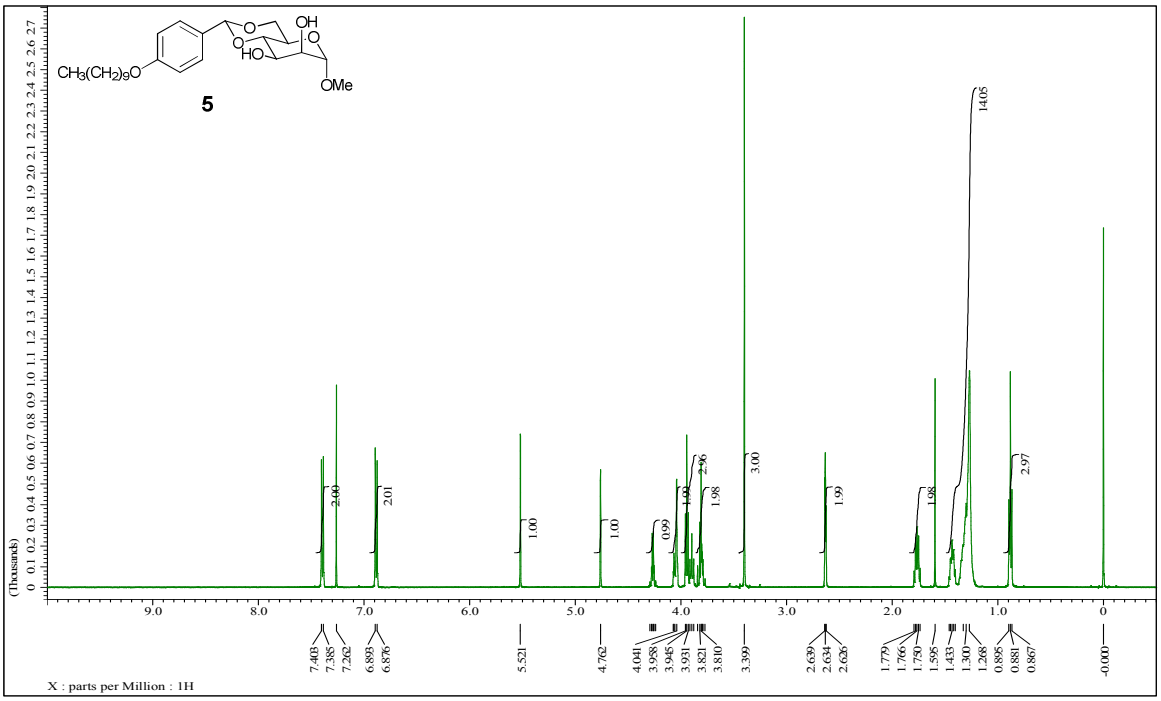

CH3(CH2)3O
OH
O
HO
OMe
2
abundance
X : parts per Million : 13C

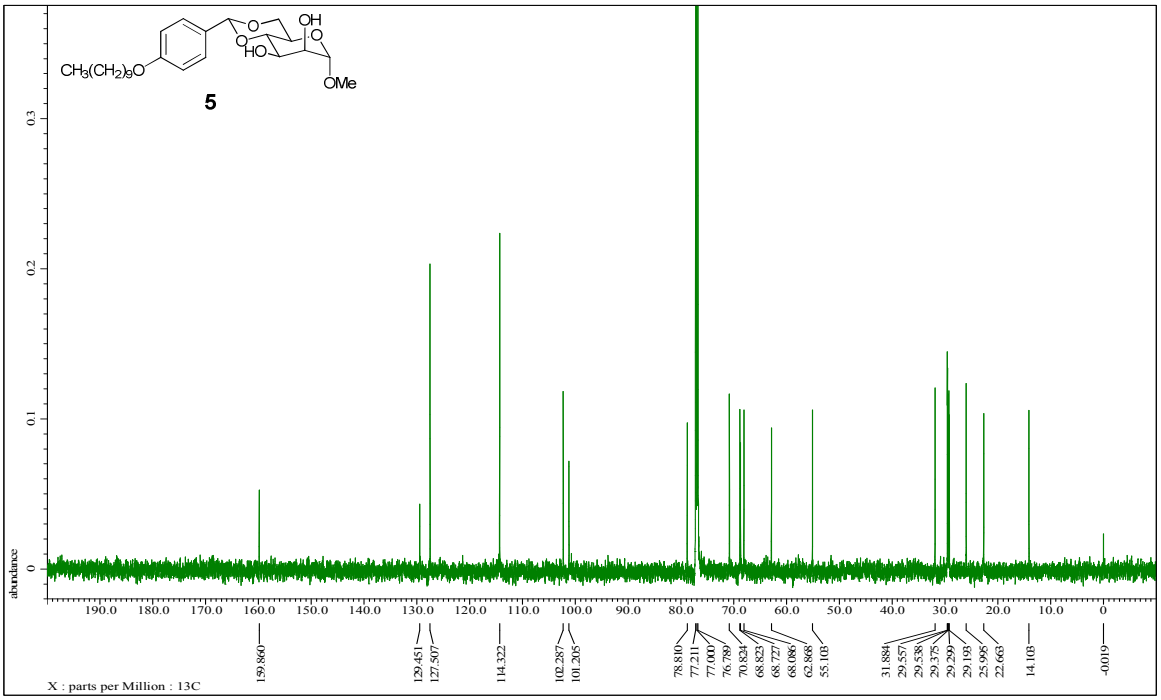

CH3(CH2)5O
OH
O
HO
OMe
3
abundance
X : parts per Million : 1H

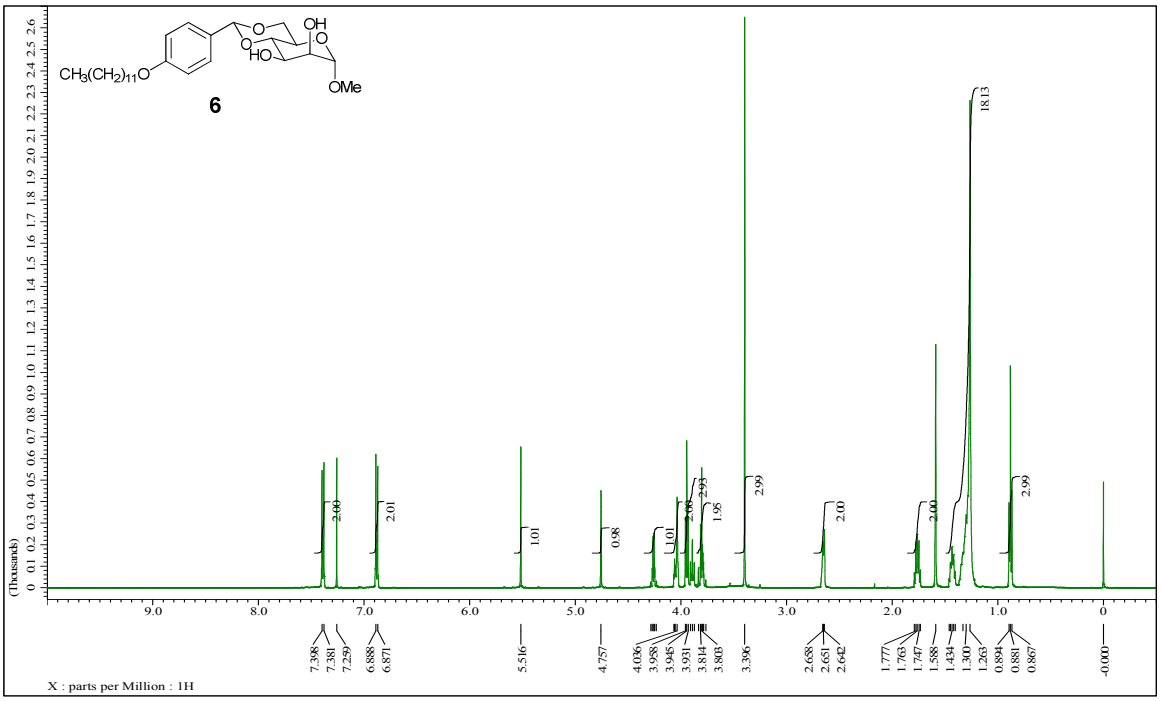

CH3(CH2)5O
OH
O
HO
OMe
3
abundance
X : parts per Million : 13C

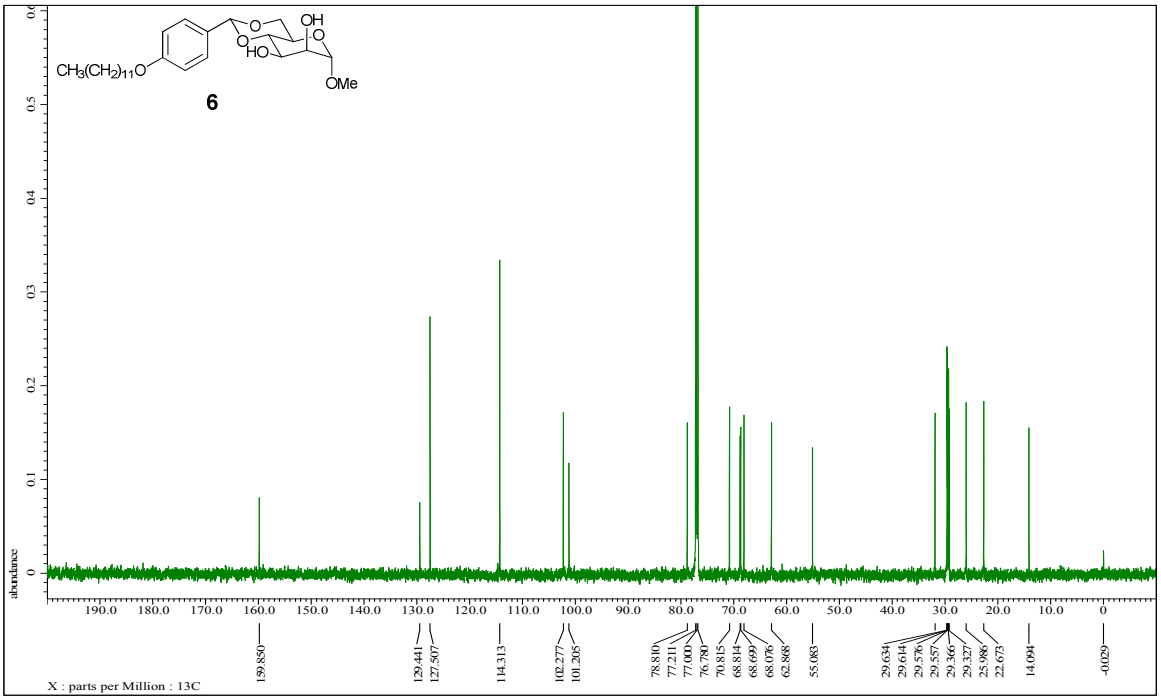

CH3(CH2)7O
OH
HO
OMe
4
abundance
X : parts per Million : 1H

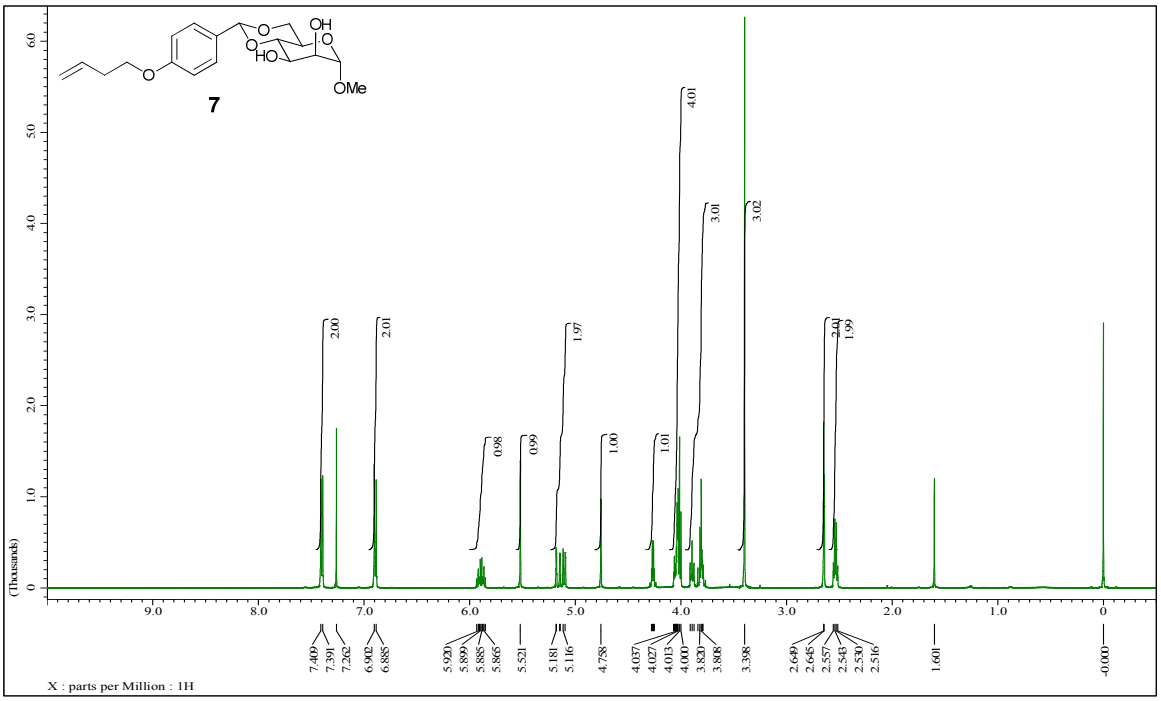

CH3(CH2)7O
OH
HO
OMe
4
abundance
X : parts per Million : 13C

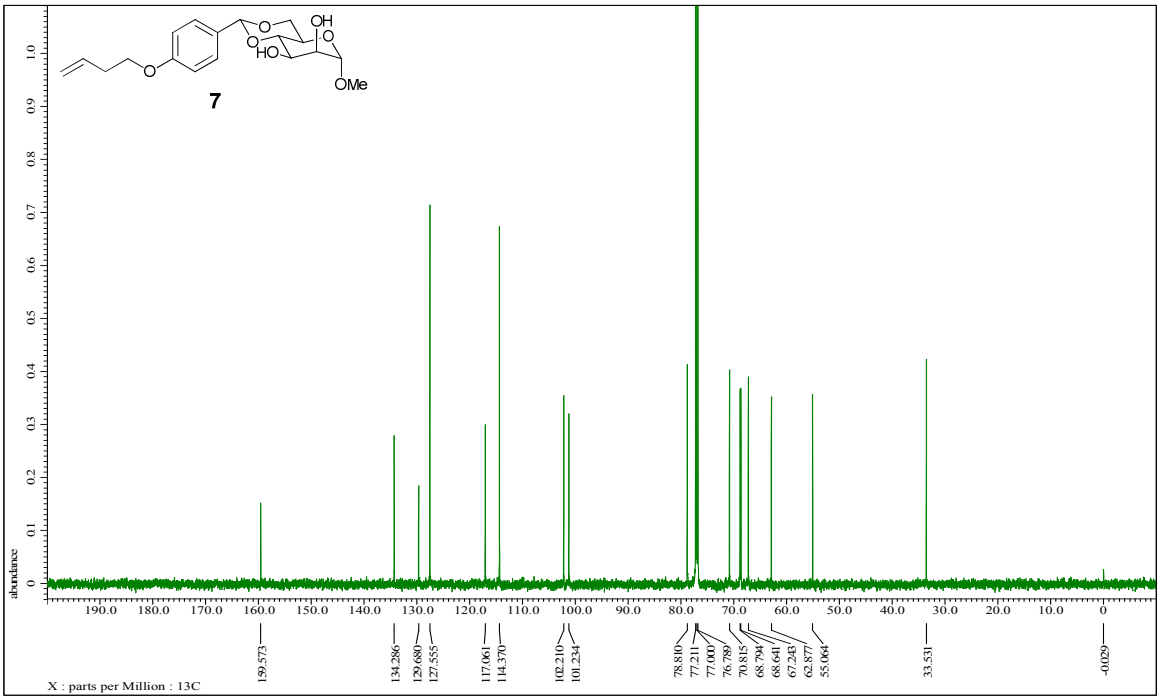

CH3(CH2)9O
OH
O
HO
OMe
5
(Thousands)
X : parts per Million : 1H

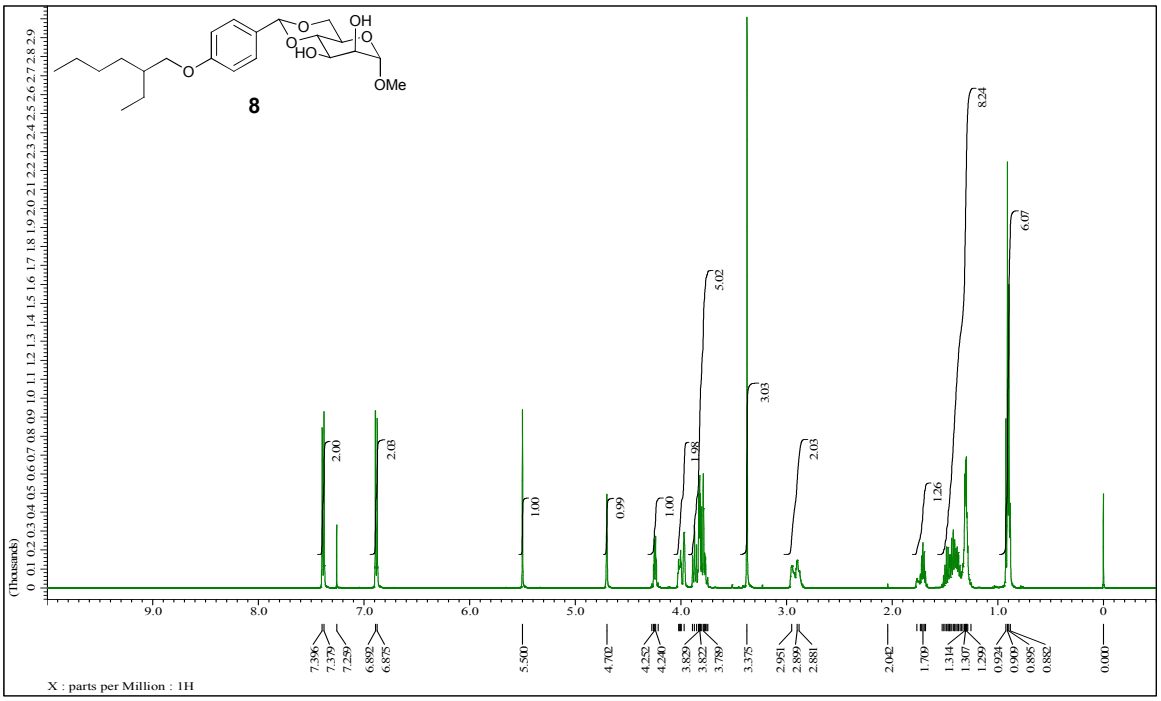

CH3(CH2)9O
OH
O
HO
OMe
5
abundance
X : parts per Million : 13C

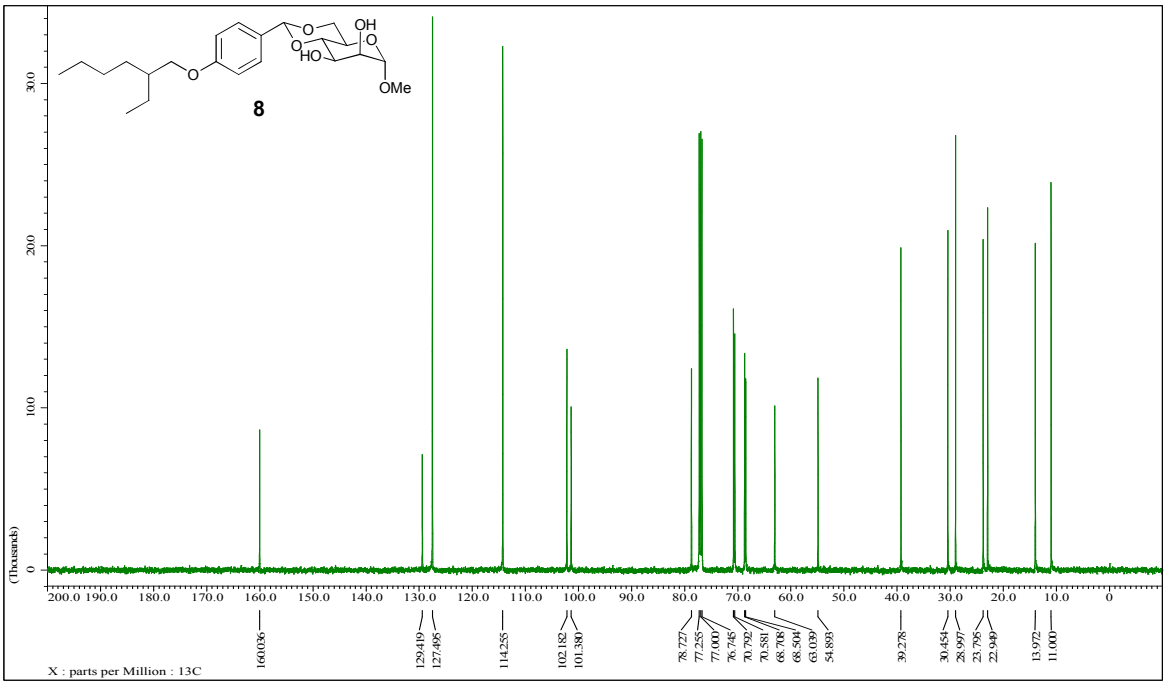

CH3(CH2)11O
OH
O
HO
OMe
6
(Thousands)
X : parts per Million : 1H

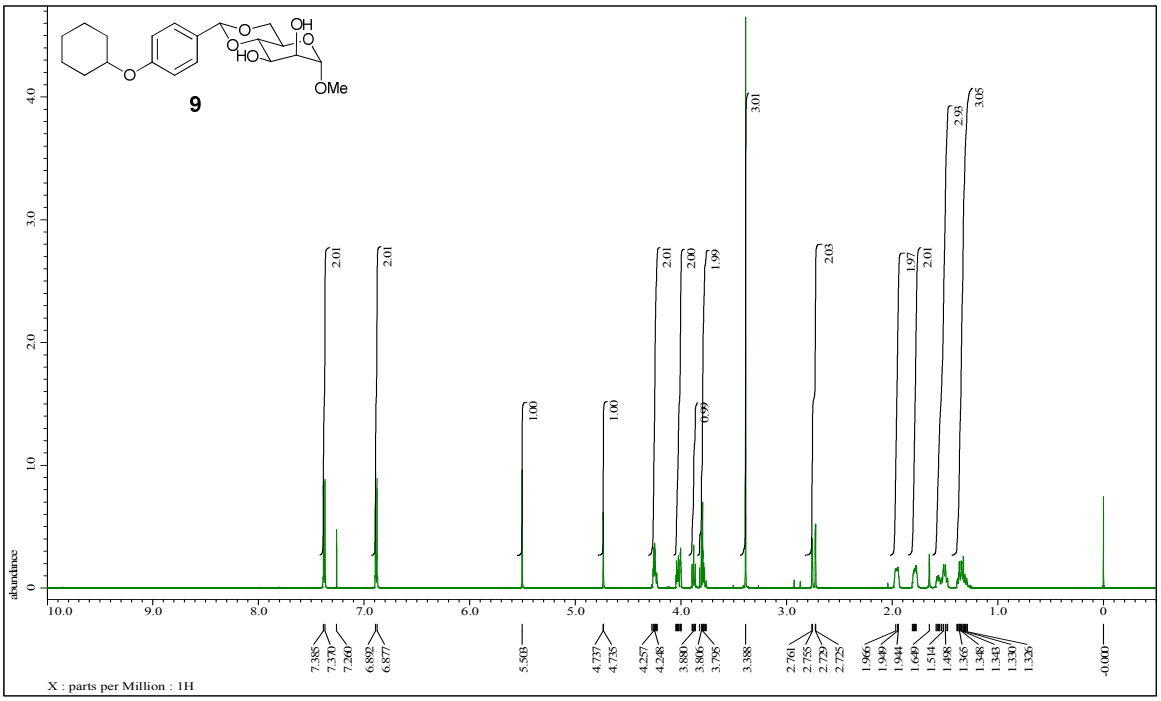

CH3(CH2)11O
OH
O
HO
OMe
6
abundance
X : parts per Million : 13C

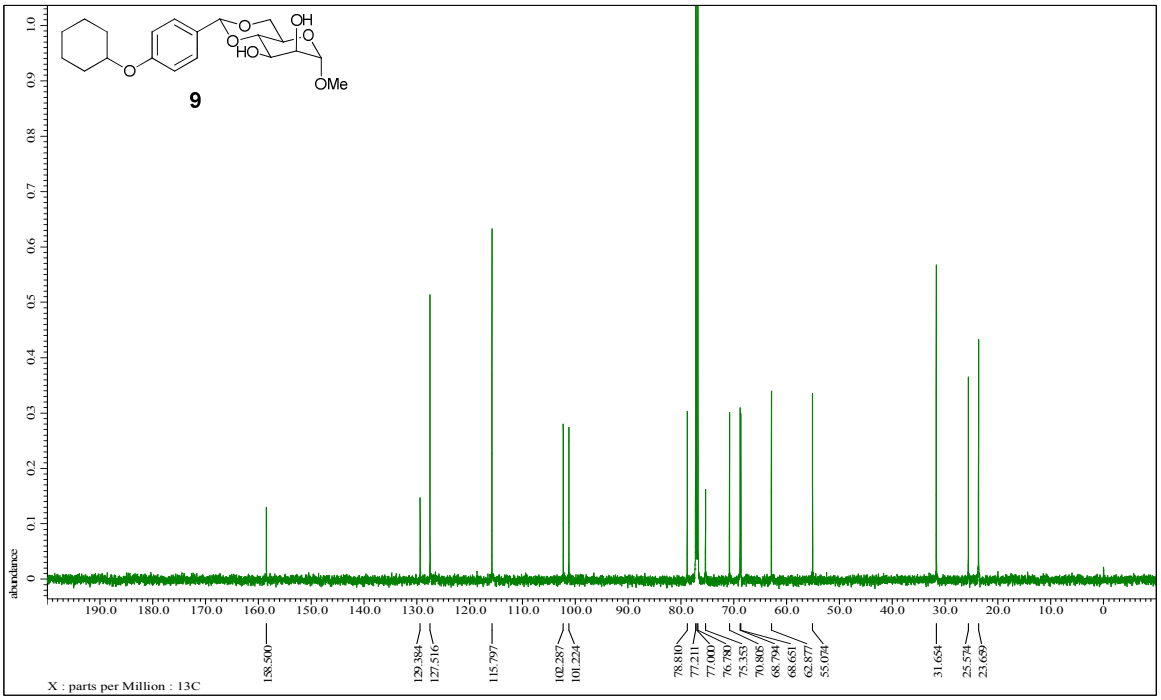

7
OH
HO
OMe
(Thousands)
X : parts per Million : 1H

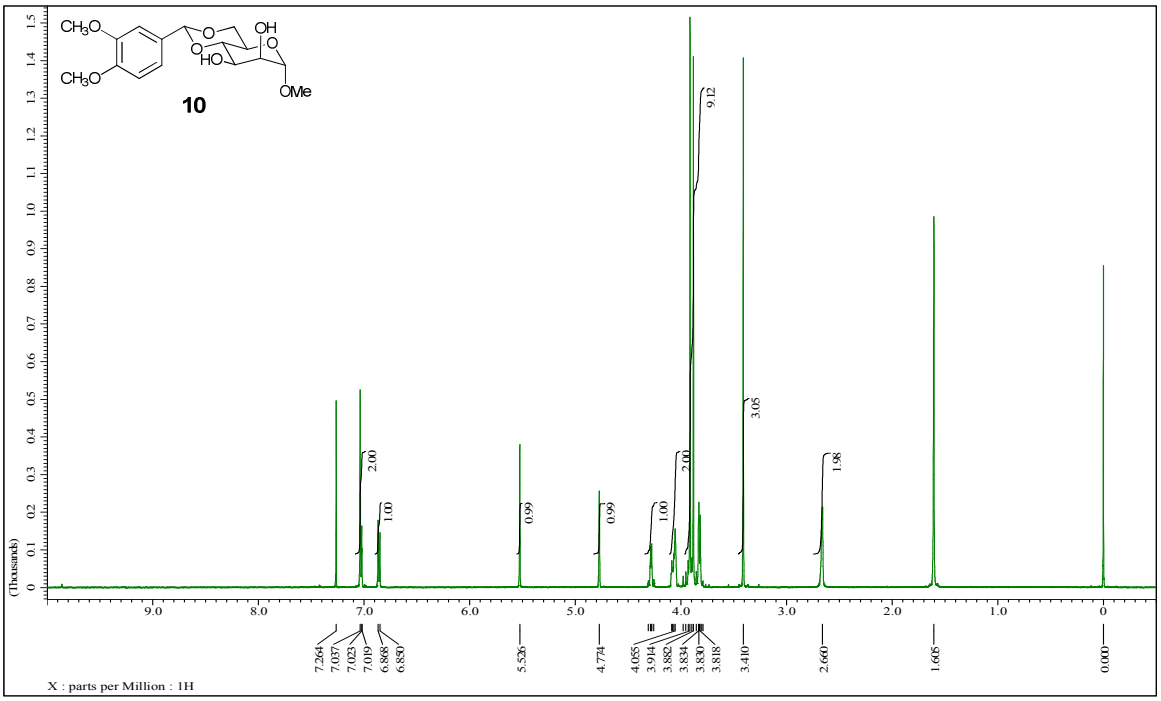

7
OH
HO
OMe
abundance
X : parts per Million : 13C

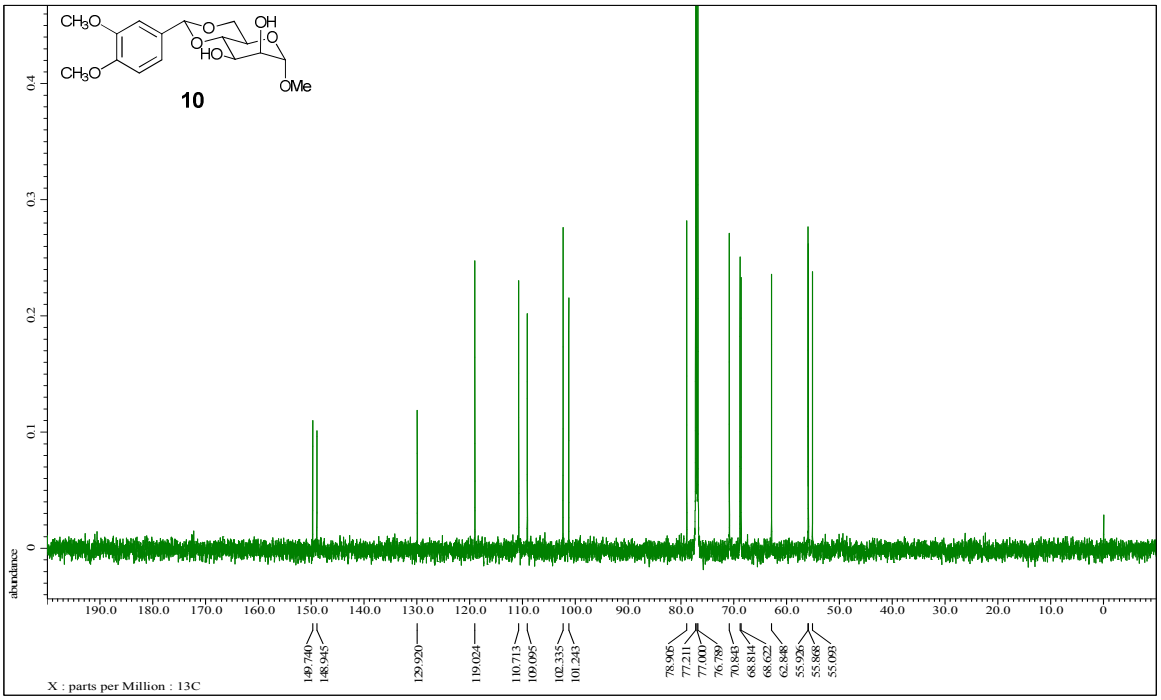

8
OH
O
HO
OMe
(Thousands)
X : parts per Million : 1H
7.396
7.379
7.259
6.892
6.875
5.500
4.702
4.252
4.240
3.829
3.822
3.789
3.375
2.951
2.899
2.881
2.042
1.709
1.314
1.307
1.299
0.924
0.909
0.895
0.882
0.000


8
OH
O
HO
OMe
(Thousands)
X : parts per Million : 13C
160.036
129.419
127.495
114.255
102.182
101.380
78.727
77.255
77.000
76.746
70.792
70.581
68.708
68.504
63.039
54.893
39.278
30.454
28.997
23.795
22.940
13.972
11.000


9
OH
O
HO
OMe
abundance
X : parts per Million : 1H


9
OH
O
HO
OMe
abundance
X : parts per Million : 13C


10
(Thousands)
X : parts per Million : 1H


10
abundance
X : parts per Million : 13C