

## Supporting Informations For

# Synthesis and Characterization of Novel Azobenzene-based Meogens and their organization at Air-water and Air-solid Interfaces

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## Analytical data of the oligomeric mesogens (4a-4h) synthesized in this study

### Compound 4a

**FT-IR** ( $\text{cm}^{-1}$ ): 3046.22 (aromatic C-H stretch), 2944.17, 2871.07 (aliphatic C-H stretch), 2226.77 (C≡N stretch), 1724.27 (C=O stretch), 1601.82, 1475.36 (C=C stretch), 1252.26 (C-O stretch).

**Raman Peaks** ( $\text{cm}^{-1}$ ): 2234, 1721, 1603, 1488, 1259.

**UV-Vis** (nm): 265.00, 325.00, 450.00.

**$^1\text{H NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.85 (t, 2H), 8.80 (d, 4H), 7.66 (m, 16H), 7.52 (d, 8H), 7.0 (d, 8H), 4.48 (t, 8H,  $J = 4, 8$  Hz), 4.07 (t, 8H,  $J = 8$  Hz), 1.96-1.27 (m, 24H).

**$^{13}\text{C NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.18, 159.59, 145.16, 132.58, 132.40, 132.17, 128.35, 127.96, 127.06, 119.12, 115.04, 110.06, 67.71, 65.67, 28.85, 28.46, 22.65.

**Elemental analysis (%)**: Calculated C 74.87 H 5.56 N 5.95. Found C 74.90 H 5.83 N 5.60.

### Compound 4b

**FT-IR** ( $\text{cm}^{-1}$ ): 3045.16 (aromatic C-H stretch), 2944.87, 2869.45 (aliphatic C-H stretch), 2223.63 (C≡N stretch), 1715.84 (C=O stretch), 1601.25, 1473.84 (C=C stretch), 1245.14 (C-O stretch).

**Raman Peaks** ( $\text{cm}^{-1}$ ): 2229, 1725, 1603, 1446, 1250.

**UV-Vis** (nm): 265.00, 332.00, 441.00.

**$^1\text{H NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.84 (t, 2H), 8.79 (d, 4H), 7.65 (m, 16H), 7.52 (d, 8H), 6.98 (d, 8H), 4.46 (t, 8H,  $J = 4, 8$  Hz), 4.04 (t, 8H,  $J = 8$  Hz), 1.91-1.27 (m, 32H).

**$^{13}\text{C NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.20, 159.67, 145.18, 132.57, 131.31, 128.32, 127.92, 127.05, 119.12, 115.02, 110.05, 67.89, 65.78, 29.72, 29.11, 28.63, 25.80.

**Elemental analysis (%)**: Calculated C 75.28 H 5.90 N 5.72. Found C 75.59 H 6.49 N 5.20.

### Compound 4c

**FT-IR** ( $\text{cm}^{-1}$ ): 3045.12 (aromatic C-H stretch), 2935.16, 2855.83 (aliphatic C-H stretch), 2226.89 (C≡N stretch), 1723.91 (C=O stretch), 1603.91, 1474.58 (C=C stretch), 1254.25 (C-O stretch).

**Raman Peaks** ( $\text{cm}^{-1}$ ): 2233, 1721, 1603, 1435, 1255.

**UV-Vis** (nm): 254.00, 329.00, 448.00.

**$^1\text{H NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.84 (t, 2H), 8.80 (d, 4H), 7.67 (m, 16H), 7.52 (d, 8H), 6.99 (d, 8H), 4.44 (t, 8H,  $J = 8$  Hz), 4.02 (t, 8H,  $J = 8, 4$  Hz), 1.86-1.27 (m, 40H).

**$^{13}\text{C NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.23, 159.71, 132.58, 132.23, 131.29, 128.33, 127.06, 115.03, 110.05, 68.00, 60.17, 34.76, 29.15, 29.03, 28.62, 25.98.

**Elemental analysis (%)**: Calculated C 75.66 H 6.21 N 5.51. Found C 75.55 H 6.34 N 5.09.

### Compound 4d

**FT-IR** ( $\text{cm}^{-1}$ ): 3075.83 (aromatic C-H stretch), 2919.48, 2854.73 (aliphatic C-H stretch), 2221.83 (C≡N stretch), 1719.06 (C=O stretch), 1600.46, 1474.22 (C=C stretch), 1253.16 (C-O stretch).

**Raman Peaks** ( $\text{cm}^{-1}$ ): 2227, 1725, 1603, 1439, 1251.

**UV-Vis** (nm): 267.00, 327.00, 434.00.

**$^1\text{H NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.84 (t, 2H), 8.80 (d, 4H), 7.67 (m, 16H), 7.52 (d, 8H), 6.98 (d, 8H), 4.43 (t, 8H,  $J = 8$  Hz), 4.01 (t, 8H,  $J = 8$  Hz), 1.88-1.27 (m, 48H).

**$^{13}\text{C NMR}$**  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.24, 159.73, 145.23, 132.58, 132.23, 131.25, 128.32, 127.91, 127.06, 119.14, 115.03, 110.02, 68.06, 65.92, 31.51, 29.25, 29.19, 28.65, 25.98, 25.92.

**Elemental analysis (%)**: Calculated C 76.04 H 6.47 N 5.32. Found C 76.18 H 6.26 N 4.75.

### **Compound 4e**

**FT-IR** (cm<sup>-1</sup>): 3066.89 (aromatic C-H stretch), 2923.31, 2851.85 (aliphatic C-H stretch), 2225.04 (C≡N stretch), 1722.52 (C=O stretch), 1601.96, 1473.60 (C=C stretch), 1247.11 (C-O stretch).

**Raman Peaks** (cm<sup>-1</sup>): 2230, 1725, 1606, 1440, 1253.

**UV-Vis** (nm): 251.00, 326.00, 450.00.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): δ 8.84 (t, 2H), 8.79 (d, 4H), 7.67 (m, 16H), 7.53 (d, 8H), 6.99 (d, 8H), 4.43 (t, 8H, J = 8 Hz), 4.01 (t, 8H, J = 4, 8 Hz), 1.88-1.27 (56H).

**<sup>13</sup>C NMR** (400 MHz, CDCl<sub>3</sub>): δ 165.26, 159.75, 145.24, 132.58, 132.25, 131.25, 128.32, 127.90, 127.06, 119.14, 115.04, 110.02, 68.10, 65.94, 29.43, 29.31, 29.20, 28.67, 26.01, 25.96.

**Elemental analysis (%)**: Calculated C 76.35 H 6.77 N 5.13. Found C 76.31 H 6.66 N 5.28.

### **Compound 4f**

**FT-IR** (cm<sup>-1</sup>): 3074.46 (aromatic C-H stretch), 2921.56, 2852.52 (aliphatic C-H stretch), 2224.91 (C≡N stretch), 1719.46 (C=O stretch), 1602.70, 1471.65 (C=C stretch), 1244.72 (C-O stretch).

**Raman Peaks** (cm<sup>-1</sup>): 2227, 1720, 1604, 1439, 1250.

**UV-Vis** (nm): 265.00, 335.00, 446.00.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): δ 8.84 (t, 2H), 8.80 (d, 4H), 7.67 (m, 16H), 7.53 (d, 8H), 7.0 (d, 8H), 4.43 (t, 8H, J = 4, 8 Hz), 4.00 (t, 8H, J = 4, 8 Hz), 1.89-1.27 (m, 64H).

**<sup>13</sup>C NMR** (400 MHz, CDCl<sub>3</sub>): δ 165.23, 159.78, 145.22, 132.97, 132.56, 132.26, 131.18, 128.30, 127.90, 127.04, 119.14, 115.05, 110.00, 68.13, 65.96, 29.51, 29.46, 29.37, 29.26, 29.23, 28.69, 26.05, 25.99.

**Elemental analysis (%)**: Calculated C 76.65 H 7.02 N 4.96. Found C 76.93 H 7.15 N 4.78.

### **Compound 4g**

**FT-IR** (cm<sup>-1</sup>): 3065.31 (aromatic C-H stretch), 2919.85, 2851.11 (aliphatic C-H stretch), 2223.99 (C≡N stretch), 1730.03 (C=O stretch), 1603.66, 1475.23 (C=C stretch), 1246.39 (C-O stretch).

**Raman Peaks** (cm<sup>-1</sup>): 2229, 1735, 1606, 1438, 1248.

**UV-Vis** (nm): 265.00, 333.00, 450.00.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): δ 8.85 (t, 2H), 8.80 (d, 4H), 7.67 (m, 16H), 7.54 (d, 8H), 7.0 (d, 8H), 4.42 (t, 8H, J = 8, 4 Hz), 4.00 (t, 8H, J = 8, 4 Hz), 1.87-1.27 (72H).

**<sup>13</sup>C NMR** (400 MHz, CDCl<sub>3</sub>): δ 165.26, 159.77, 145.26, 132.58, 132.26, 131.24, 128.32, 127.90, 127.06, 115.05, 110.02, 68.14, 65.97, 29.52, 29.40, 29.28, 29.22, 28.68, 26.04, 25.98.

**Elemental analysis (%)**: Calculated C 76.94 H 7.26 N 4.80. Found C 76.43 H 7.37 N 4.48.

### **Compound 4h**

**FT-IR** (cm<sup>-1</sup>): 2957.91 (aromatic C-H stretch), 2922.32, 2851.62 (aliphatic C-H stretch), 2224.68 (C≡N stretch), 1718.73 (C=O stretch), 1603.49, 1468.27 (C=C stretch), 1256.86 (C-O stretch).

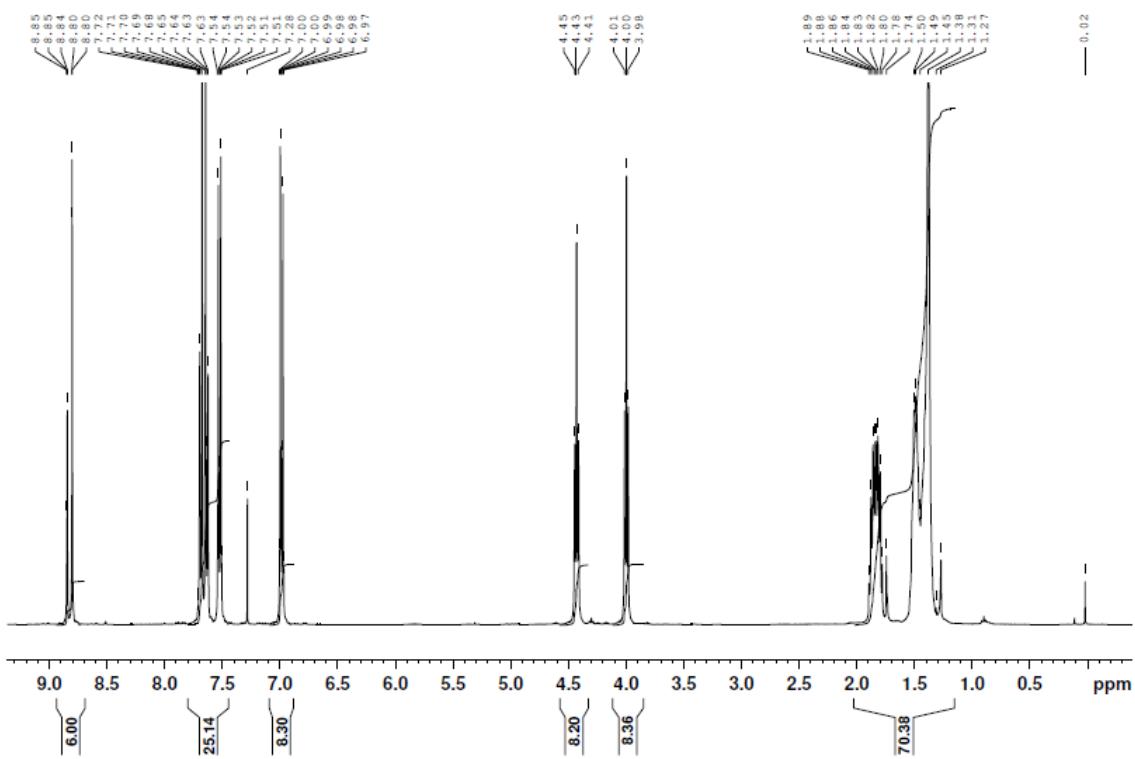
**Raman Peaks** (cm<sup>-1</sup>): 2236, 1725, 1607, 1447, 1249.

**UV-Vis** (nm): 265.00, 333.00, 442.00.

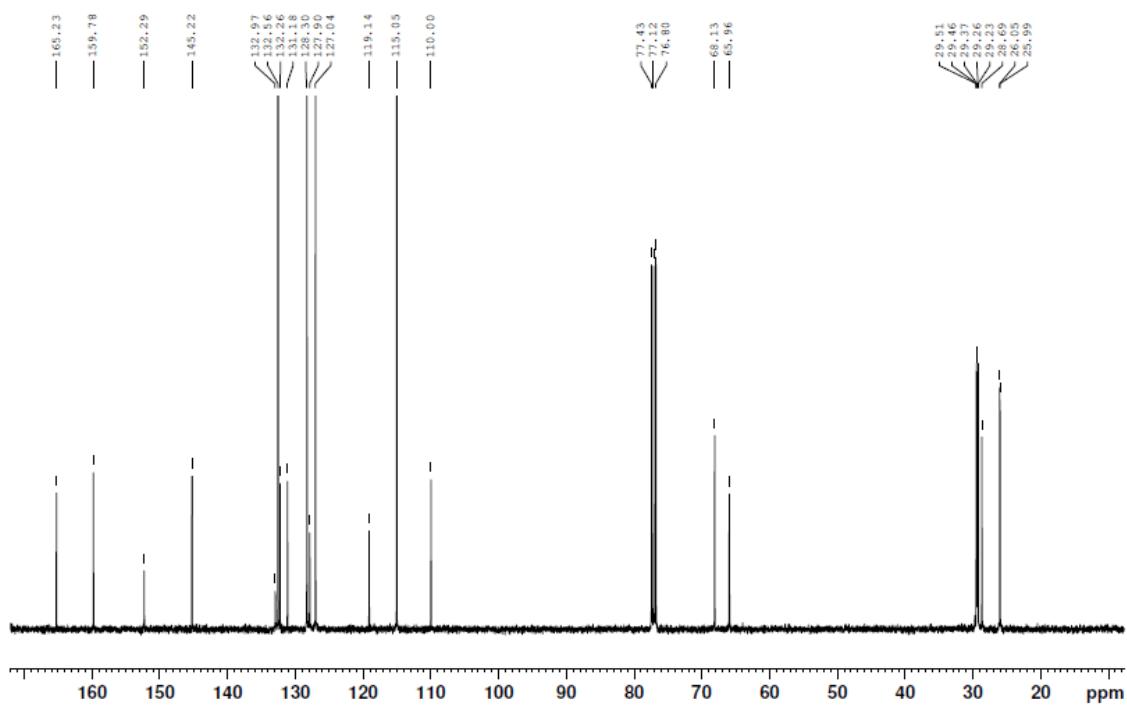
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): δ 8.84 (t, 2H), 8.80 (d, 4H), 7.67 (m, 16H), 7.54 (d, 8H), 7.0 (d, 8H), 4.42 (t, 8H, J = 8, 4 Hz), 4.01 (t, 8H, J = 4, 8 Hz), 1.89-1.28 (m, 80H).

**<sup>13</sup>C NMR** (400 MHz, CDCl<sub>3</sub>): δ 165.26, 159.78, 145.26, 132.58, 132.26, 131.23, 128.32, 127.90, 127.06, 119.14, 115.05, 110.02, 68.15, 65.97, 29.58, 29.54, 29.41, 29.29, 29.23, 28.69, 26.05, 25.99.

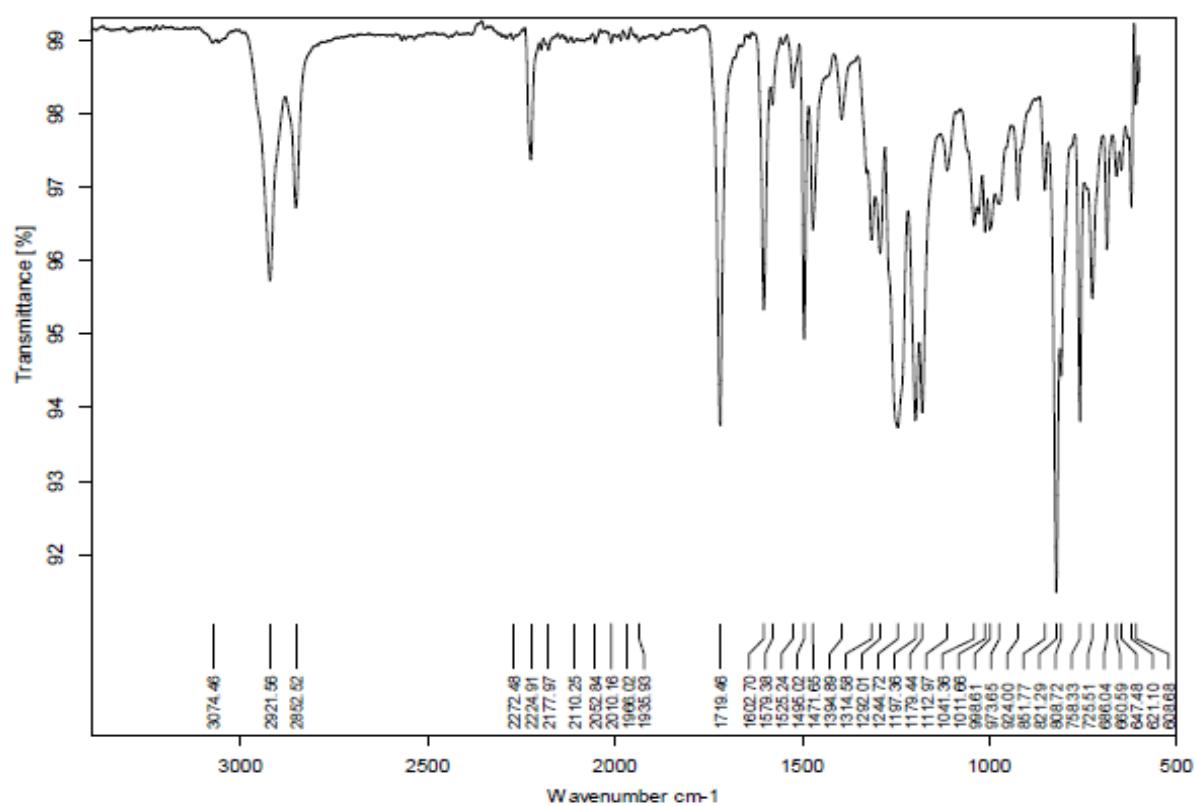
**Elemental analysis (%)**: Calculated C 77.21 H 7.48 N 4.65. Found C 77.28 H 7.66 N 4.64.



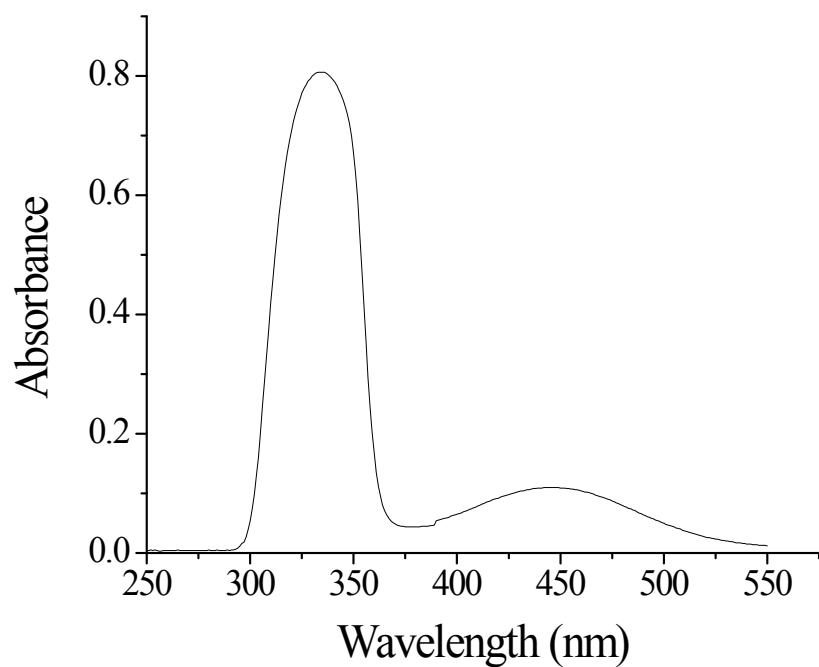
**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **4f**.



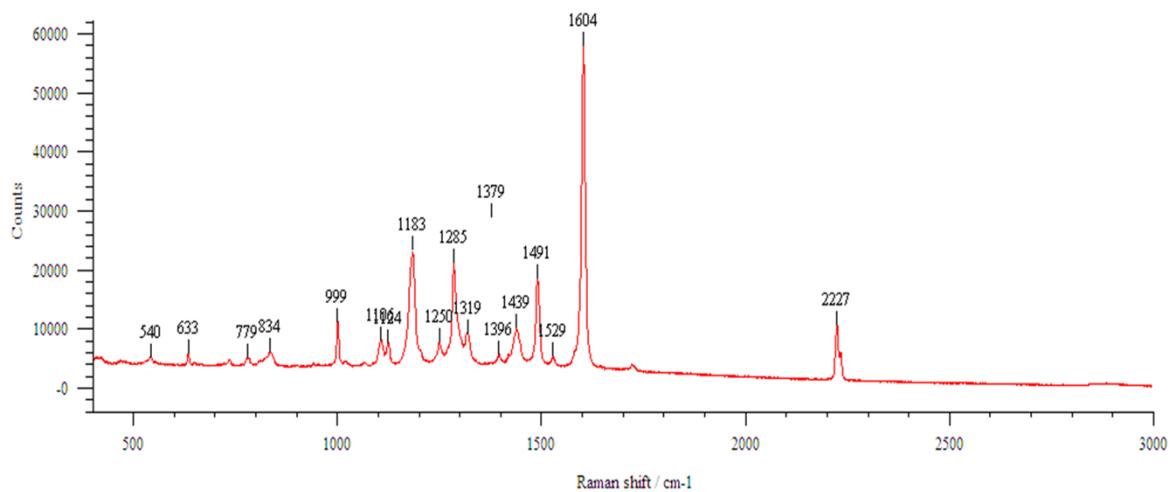
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of compound **4f**.



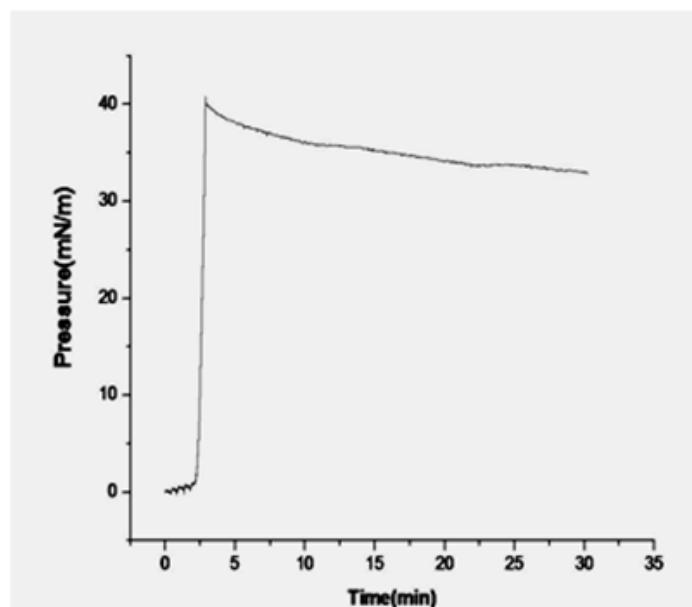
**Figure S3.** IR spectrum of compound **4f**.



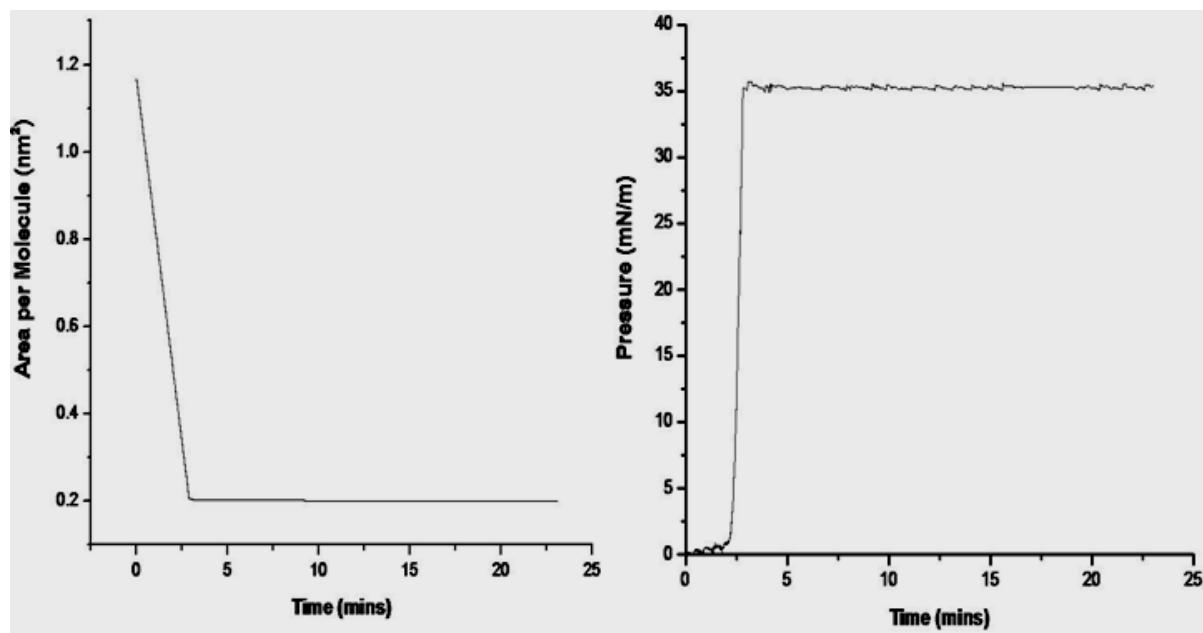
**Figure S4.** UV-Vis spectrum of compound **4f**.



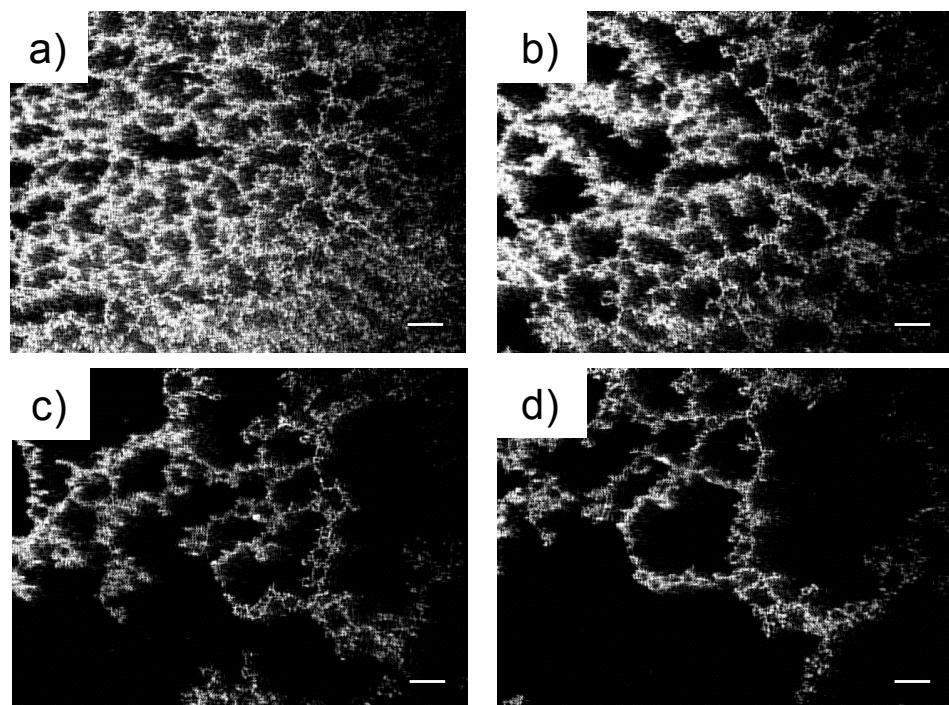
**Figure S5.** Raman spectrum of compound **4f**.



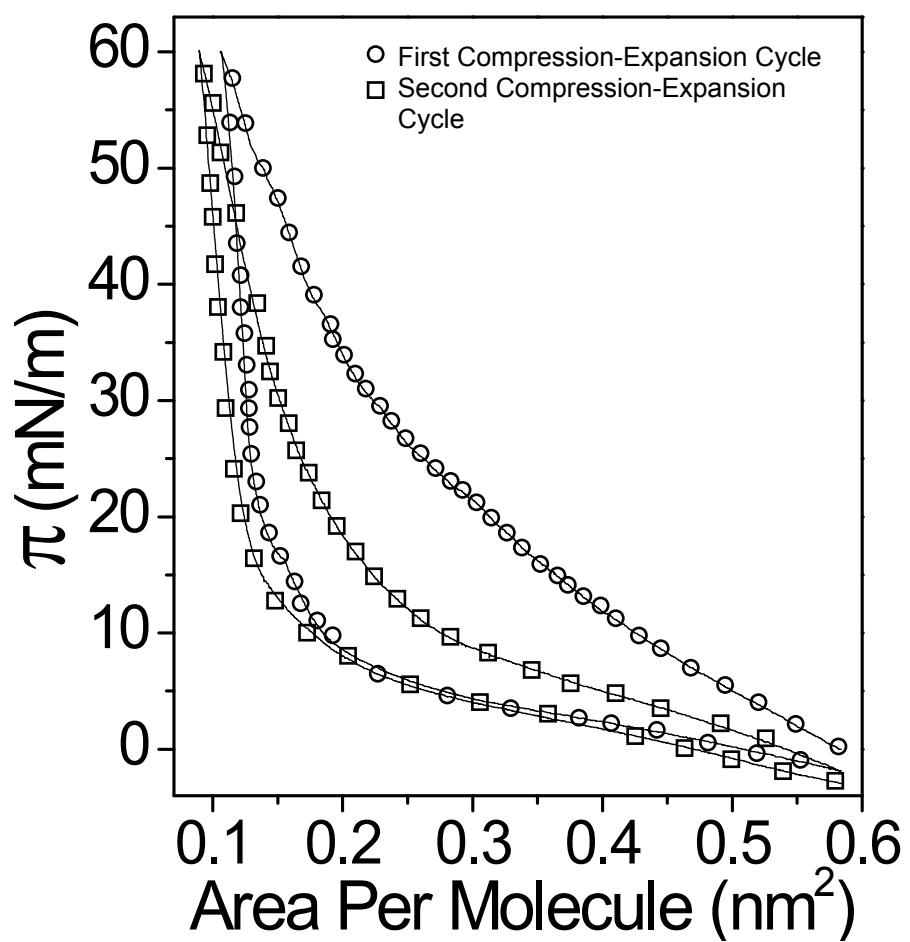
**Figure S6.** Equilibrium surface pressure measurement (for compound **4f** at air-water interface) by keeping the barriers constant.



**Figure S7.** For stability measurement of the film of compound **4f** at air-water interface control pressure (35 mN/m) was setup and the variation of area per molecule with time was observed to keep the pressure constant.



**Figure S8.** BAM images of expansion for compound **4f** at air-water interface. The area per molecule in each case is (a)  $0.4 \text{ nm}^2$  (b)  $0.5 \text{ nm}^2$  (c)  $0.6 \text{ nm}^2$  (d)  $0.8 \text{ nm}^2$ . Scale bar in each case is  $500 \mu\text{m}$ .



**Figure S9.** The plot shows prominent hysteresis for compression-expansion  $\pi$ - $A_m$  cycles of compound **4f** at air-water interface.