SUPPLEMENTARY MATERIALS

Formation and Thermal Stability of Ordered Self-Assembled Monolayers by Adsorption of Amide-Containing Alkanethiols on Au(111)

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1. Synthesis of N-(2-mercaptoethyl)heptanamide (MEHA)

1.1. Materials

Heptanoic acid (≥99.0%, Sigma-Aldrich), N-hydroxysuccinimide (NHS; ≥98.0%, TCI), N, N'-dicyclohexylcarbodiimide (DCC; ≥98.0%, TCI), Dichloromethane (DCM; ≥99.8%, Sigma-Aldrich), 2-Aminoethanethiol (≥95.0%, TCI), and triethylamine (≥99.0%, Sigma-Aldrich) were purchased and used without further purification.

1.2. Synthesis of MEHA

2,5-dioxopyrrolidin-1-yl heptanoate: At 0 °C, DCC (6.190 g, 30 mmol) was added to a dioxane solution (500 mL) containing heptanoic acid (3.9056 g, 30 mmol) and NHS (3.452 g, 30 mmol), and the mixture was stirred at 20 °C overnight. 2,5-dioxopyrrolidin-1-yl heptanoate, a white solid obtained by evaporating the reaction mixture, was then used for the subsequent procedure without further purification.

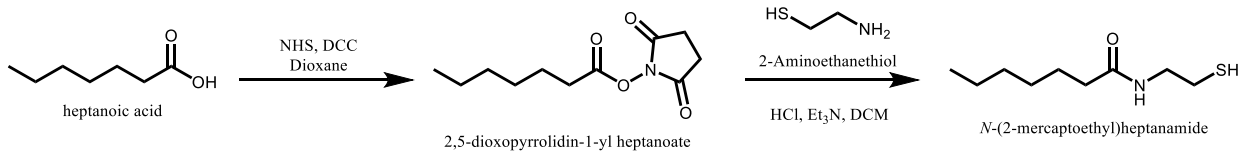

Figure S1. Synthetic schematic illustration of MEHA

N-(2-mercaptoethyl)heptanamide (MEHA): 2,5-dioxopyrrolidin-1-yl heptanoate and triethylamine (8.31 mL, 60 mmol) were added to a DCM solution (350 mL) and stirred for 4 h at 20 °C.

The reaction mixture was washed twice in 100 mL of 1 N aqueous HCl, dried over Na_2SO_4, and then evaporated to dryness. The residue was purified with an eluent (hexane: EA=1:1) over silica gel, and the second layer was isolated from the column and evaporated to produce MEHA as a white solid (1.4114 g, 24.9 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 5.832 (br, 1H), 3.463-3.416 (q, 2H), 2.212-2.174 (t, 2H), 1.672-1.598 (m, 2H), 1.356-1.242 (m, 7H), 0.902-0.868 (t, 3H).

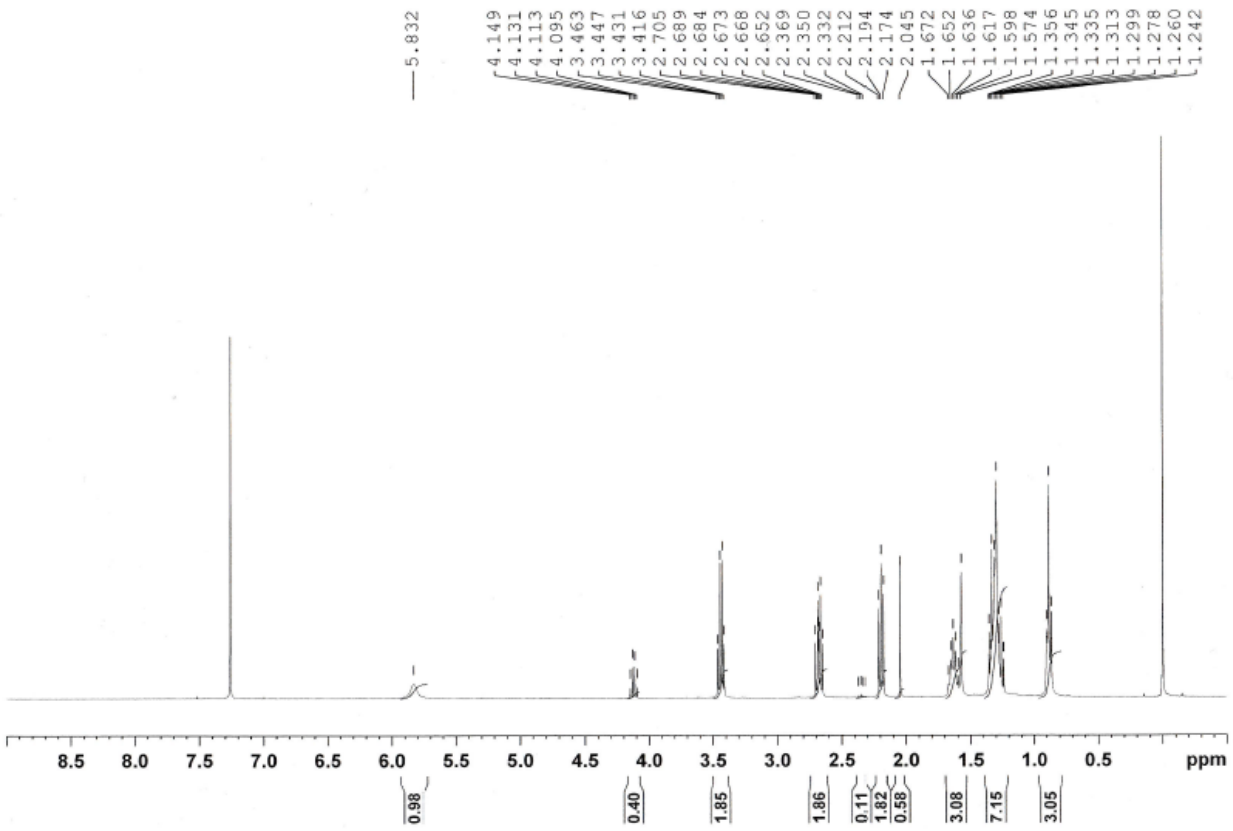

Figure S2. H[1] NMR Spectrum (400 MHz, $CDCl_3$) of MEHA.