

**Supplemental Information** to “LCD-based detection of enzymatic action” by Johan Hoogboom, Kelly Velonia, Theo Rasing, Alan E. Rowan and Roeland J.M. Nolte

To a cooled amount of  $\gamma$ -aminopropyl-triethoxysilane (1.1 ml, 4.6 mmole) was added maleic anhydride (0.45 g, 4.6 mmole), after which **1** was formed in a vigorous reaction as a solid white product in quantitative yield. A solution of **1** (1.47 g, 4.6 mmole) in 10 ml of chloroform was added dropwise to a solution of benzyl alcohol (0.5 g, 4.6 mmole) and dicyclohexyl-carbodiimide (0.95 g, 4.6 mmole) in 20 ml of chloroform, containing a catalytic amount of N-N'-dimethylaminopyridine. After stirring for 1 hr, the mixture was filtered and the solvent removed under vacuum. Repeated recrystallisations from hexane yielded compound **2** as a white solid in a yield of 62%.

**1**:  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ , 20°C, TMS):  $\delta$  = 8.34 (br, 1H, OH), 6.46 (d,  $J$  = 12.9 Hz, 1H, HN(CO)CH), 6.26 (d,  $J$  = 12.8 Hz, 1H, HCCOOH), 3.78 (q,  $J$  = 7.1 Hz, 6H,  $\text{OCH}_2\text{CH}_3$ ), 3.33 (m, 2H, HNCH<sub>2</sub>), 1.70 (m, 2H,  $\text{CH}_2\text{-CH}_2\text{-CH}_2$ ), 1.19 (t,  $J$  = 7.1 Hz, 9H, CH<sub>3</sub>), 0.63 (m, 2H, Si-CH<sub>2</sub>).

$^{13}\text{C}\{^1\text{H}\}$ -NMR (50 MHz,  $\text{CDCl}_3$ , 20°C, TMS):  $\delta$  = 167.2 (s, 1C, COOH), 166.7 (s, 1C, (CO)NH), 136 (s, 1C, HN(CO)CH), 133 (s, 1C, HCCOOH), 59 (s, 3C,  $\text{OCH}_2\text{CH}_3$ ), 43 (s, 1C, HNCH<sub>2</sub>), 23 (s, 1C,  $\text{CH}_2\text{-CH}_2\text{-CH}_2$ ), 19 (s, 3C, CH<sub>3</sub>), 8 (s, 1C, Si-CH<sub>2</sub>).

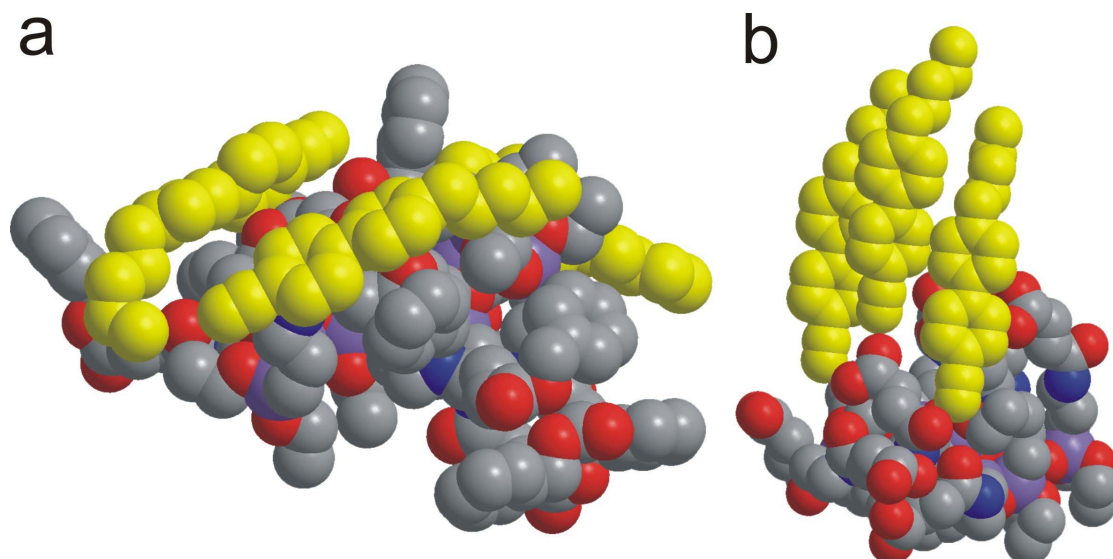
IR (KBr):  $\nu$  ( $\text{cm}^{-1}$ ) = 3319(NH), 3059 (OH), 1753 (COOH-stretch), 1662 (Amide-I), 1535 (Amide-II).

**2**:  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ , 20°C, TMS):  $\delta$  = 7.82-7.76 (m, 2H, *m*-Ph-H), 7.21-7.12 (m, 2H, *o*-Ph-H), 6.72 (m, 1H, *p*-Ph-H), 6.52 (d,  $J$  = 12.9 Hz, 1H, HN(CO)CH), 6.36 (d,  $J$  = 12.8 Hz, 1H, HCCOCH<sub>2</sub>), 5.92 (br, 1H, NH), 5.18 (br, 2H,  $\text{CH}_2\text{-Ph}$ ), 3.82 (q,  $J$  = 7.1 Hz, 6H,  $\text{OCH}_2\text{CH}_3$ ), 3.39 (m, 2H, HNCH<sub>2</sub>), 1.71 (m, 2H,  $\text{CH}_2\text{-CH}_2\text{-CH}_2$ ), 1.19 (t,  $J$  = 7.1 Hz, 9H, CH<sub>3</sub>), 0.63 (m, 2H, Si-CH<sub>2</sub>).

$^{13}\text{C}\{^1\text{H}\}$ -NMR (75 MHz,  $\text{CDCl}_3$ , 20°C, TMS):  $\delta$  = 168 (s, 1C, NH(CO)), 167 (s, 1C, (CO)CH<sub>2</sub>), 139 (s, 1C, *ipso*-Ph-C), 138 (s, 1C, HN(CO)CH), 137 and 136 (s, 2C, Ph-C), 135 (s, 1C, HCCOOH), 130 (s, 1C, Ph-C), 67 (s, 1C,  $\text{CH}_2\text{-Ph}$ ), 58 (s, 3C,  $\text{OCH}_2\text{CH}_3$ ), 46 (s, 1C, HNCH<sub>2</sub>), 23 (s, 1C,  $\text{CH}_2\text{-CH}_2\text{-CH}_2$ ), 20 (s, 3C, CH<sub>3</sub>), 8 (s, 1C, Si-CH<sub>2</sub>).

IR (KBr):  $\nu$  ( $\text{cm}^{-1}$ ) = 3325(NH), 1658 (Amide-I), 1542 (Amide-II).

Due to the oligomerization of **1** and **2**, no elemental analysis could be obtained.



**Figure S1: Schematic representation of a minimum-energy conformation of the alignment layer and mesogen. a) Before hydrolysis. b) After hydrolysis. Shown is a pentamer of the siloxane in interaction with 3 molecules of 5CB (yellow). Minimum energy structures were obtained by at least three cycles of molecular dynamics-energy minimisation at the MM2 level, followed by an energy minimisation at the PM3 level. (Chem3D Ultra 9.0, ©Cambridgesoft 2004)**