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 γ-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: $^1$H-NMR (300 MHz, CDCl$_3$, 20°C, TMS): δ = 8.34 (br, 1H, OH), 6.46 (d, $J = 12.9$ Hz, 1H, HN(CO)CH$_2$), 6.26 (d, $J = 12.8$ Hz, 1H, HCCOOH), 3.78 (q, $J = 7.1$ Hz, 6H, OCH$_2$CH$_3$), 3.33 (m, 2H, HNC$_2$H$_4$), 1.70 (m, 2H, CH$_2$-CH$_2$-CH$_2$), 1.19 (t, $J = 7.1$ Hz, 9H, CH$_3$), 0.63 (m, 2H, Si-CH$_2$).

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

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

2: $^1$H-NMR (300 MHz, CDCl$_3$, 20°C, TMS): δ = 7.82-7.76 (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, HCCOOCH$_2$), 5.92 (br, 1H, NH), 5.18 (br, 2H, CH$_2$-Ph), 3.82 (q, $J = 7.1$ Hz, 6H, OCH$_2$CH$_3$), 3.39 (m, 2H, HNC$_2$H$_4$), 1.71 (m, 2H, CH$_2$-CH$_2$-CH$_2$), 1.19 (t, $J = 7.1$ Hz, 9H, CH$_3$), 0.63 (m, 2H, Si-CH$_2$).

$^{13}$C{1H}-NMR (75 MHz, CDCl$_3$, 20°C, TMS): δ = 168 (s, 1C, NH(CO)), 167 (s, 1C, (CO)CH$_2$), 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, CH$_2$-Ph), 58 (s, 3C, OCH$_2$CH$_3$), 46 (s, 1C, HNCH$_2$), 23 (s, 1C, CH$_2$-CH$_2$-CH$_2$), 20 (s, 3C, CH$_3$), 8 (s, 1C, Si-CH$_2$).

IR (KBr): ν (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)