Electronic Supplementary Material (ESI) for RSC Advances.

1. Experimental

1.1. General Methods

4-Hydroxy-4′-nitrobiphenyl was prepared as described previously. [1] Miscellaneous solvents were purchased from Fisher Scientific dried by sequential percolation through columns of activated alumina and copper Q5 catalyst prior to use. Reactions were monitored by thin layer chromatography (TLC) using an appropriate solvent system. Silica coated aluminium TLC plates used were purchased from Merck (Kieselgel 60 F-254) and visualised using visible light (both starting materials and products are yellow) and UV light at 254 nm Column chromatography was performed using flash grade silica from Fluorochem (40 - 63μm particle size). Yields refer to chromatographically (HPLC) and spectroscopically (^{1}H NMR, ^{13}C{^{1}H} NMR) homogenous material.

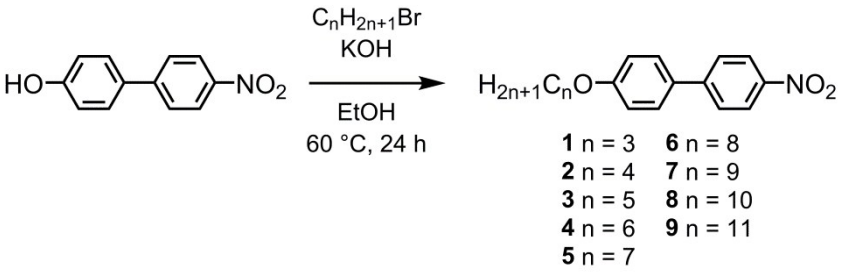
NMR spectra were recorded on a JEOL ECS spectrometer operating at 400 MHz (^{1}H), 100.5 MHz (^{13}C{^{1}H}) and 376.4 MHz (^{19}F NMR) as solutions in deuterated chloroform. Mass spectra were recorded on a Bruker micrOTOF MS-Agilent series 1200LC spectrometer. FTIR spectroscopy was performed using a Shimadzu IR Prestige-21 with Specac Golden Gate diamond ATR IR insert that was flushed with nitrogen prior to use. High-performance liquid chromatography was performed on a Shimadzu Prominence modular HPLC system comprising a LC-20A quaternary solvent pump, a DGU-20A$_5$ degasser, a SIL-20A autosampler, a CBM-20A communication bus, a CTO-20A column oven, and a SPO-20A dual wavelength UV-vis detector operating at 220/250 nm. The column used was an Alltech C18 bonded reverse-phase silica column with a 5 μm pore size, an internal diameter of 10 mm and a length of 250 mm. In all cases the mobile phase used was neat acetonitrile, purchased from Fisher Scientific UK.

Polarised optical microscopy was performed on a Zeiss Axioskop 40Pol microscope using a Mettler FP82HT hotstage controlled by a Mettler FP90 central processor. Photomicrographs were captured *via* an InfinityX-21 MP digital camera mounted atop the microscope. Differential scanning calorimetry was performed on a Mettler DSC822^{e} fitted with an autosampler operating with Mettler Star^{e} software and calibrated before use against an indium standard (onset = 156.55 ± 0.2 °C, ΔH = 28.45 ± 0.40 Jg^{-1}) under an atmosphere of dry nitrogen.

Small angle X-ray diffraction was performed using a Bruker D8 Discover equipped with a temperature controlled, bored graphite rod furnace, custom built at the University of York. The radiation used was copper Kα (λ = 0.154056 nm) from a 1 μS microfocus source. Diffraction patterns were recorded on a 2048x2048 pixel Bruker VANTEC 500 area detector set at a distance of 121 mm from the sample. Samples were filled into 1mm capillary tubes

and aligned with a pair of 1T magnets, with the field strength at the sample position being approximately 0.6T Diffraction patterns were collected as a function of temperature and the data processed using Matlab. Quantum chemical calculations were performed using the Gaussian 09 revision e.01 suite of programmes. [2]

In order to assess the behaviour of the materials under applied electric fields, cells were placed within a Metter FP82HT hotstage, which was controlled by a Mettler FP90 temperature controller. The hotstage was mounted on a Ziess Universal polarizing microscope, fitted with an 8/0.2 objective and x10 widefield eyepieces. The waveform was generated by a Hewlett Packard 33120A arbitrary waveform generator and amplified by a linear x20 amplifier that was custom built by QinetiQ. The electrical response from the cell was amplified by a nano-current amplifier (20 kΩ or 100 kΩ impedance) and fed into a Hewlett Packard 54600B oscilloscope, which was connected to a PC. The antiparallel buffed polyimide cells used (Halation) had spacings of approx. 50 μm, and were constructed from ITO-coated glass. In all cases, the cells were filled by capillary action at atmospheric pressure with the sample in the isotropic liquid at 85 °C. Wires were affixed to the cells using neat indium metal as a solder. To determine the threshold voltage the cell was subjected to an applied field of 1 V at a frequency of 1 Hz and the voltage increased in increments of 1 V until the area sandwiched between the ITO electrodes became entirely optically extinct. Increasing the frequency of the applied field to 20 KHz afforded a transformation into a scattering state.



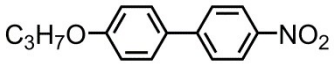
Scheme 1

1.2. General Alkylation Procedure

4-Hydroxy-4′-nitrobiphenyl (1 mol eqv.), bromohalide (1.5 mol eqv.) and KOH (1.5 mol eqv.) were dissolved into ethanol with vigorous stirring and heated to 60 °C (internal temperature) for 24 hours. Reactions were monitored by TLC, with the consumption of 4-hydroxy-4′-

nitrobiphenyl (Rf_{DCM} = 0.1) and the formation of the 4-alkoxy-4′-nitrobiphenyl (Rf_{DCM} = 0.45) taken to be indicative of a complete reaction. Once complete the reaction solution was chilled, precipitating the crude product. The precipitate was collected, dissolved into dichloromethane and purified by flash chromatography with a gradient of DCM/hexanes. The chromatographed materials were recrystalised from hexanes, affording the title compounds as pale yellow crystalline solids.

1.3. Chemical Characterisation



1: 4-Propyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl (1.0 g, 4.65 mmol), bromopropane (0.85 g, 0.63 ml 6.97 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 0.7 g (58%)

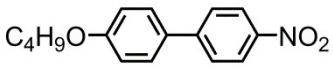
^{1}H NMR (400 MHz, $CDCl_3$): 0.99 (3H, t, *J* = 7.3, CH_3), 1.77 (2H, sext, *J* = 7.3, CH_2), 3.91 (2H, t, *J* = 7.3, CH_2O), 6.93 (2H, ddd, *J* = 2.2, *J* = 2.9, *J* = 8.8, Ar), 7.49 (2H, ddd, *J* = 2.2, *J* = 2.9, *J* = 8.8, Ar), 7.61 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar), 8.19 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 10.60, 22.63, 69.71, 115.21, 124.23, 127.10, 128.61, 130.89, 146.56, 147.36, 160.12

IR (v_{max} cm^{-1}): 509, 547, 624, 694, 817, 840, 910, 1010, 1041, 1103, 1172, 1242, 1327, 1465, 1504, 1597, 1720, 2877, 2939

MS m/z (mTOF, ESI+): 280.0926 ($C_{15}H_{15}NNaO_3$, M+Na), 258.1114 (100%, $C_{15}H_{16}NO_3$, M+H)

Assay (HPLC): 99.6%



2: 4-Butyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl (1.0 g, 4.65 mmol), bromobutane (0.99 g, 0.79 ml 6.97 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 0.5 g (39%)

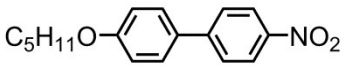
^{1}H NMR (400 MHz, $CDCl_3$): 0.97 (3H, t, *J* = 7.3, CH_3), 1.48 (2H, sext, *J* = 7.3, CH_2), 1.79 (2H, qnt, *J* = 7.3, CH_2), 3.99 (2H, t, *J* = 7.3, CH_2O), 6.98 (2H, ddd, *J* = 2.2, *J* = 3.3, *J* = 8.8, Ar), 7.54 (2H, ddd, *J* = 2.2, *J* = 3.3, *J* = 8.8, Ar), 7.66 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar), 8.23 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 13.80, 19.17, 30.89, 67.78, 115.02, 124.07, 126.94, 128.45, 130.67, 146.35, 147.20, 159.96

IR (v_{max} cm^{-1}): 501, 624, 694, 756, 833, 964, 1002, 1033, 1103, 1172, 1242, 1327, 1396, 1504, 1597, 1720, 2870, 2939

MS m/z (mTOF, ESI+): 294.1081 ($C_{16}H_{17}NNaO_3$, M+Na), 272.1270 (100%, $C_{16}H_{18}NO_3$, M+H)

Assay (HPLC): 99.2%



3: 4-Pentyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl (1.0 g, 4.65 mmol), bromopentane (1.09 g, 0.89 ml 6.97 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 1.12 g (90%)

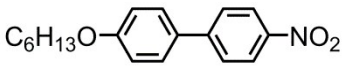
^{1}H NMR (400 MHz, $CDCl_3$): 0.87 (3H, t, *J* = 7.0, CH_3), 1.28 - 1.44 (4H, m, CH_2CH_2), 1.75 (2H, qnt, *J* = 7.0, CH_2), 3.94 (2H, t, *J* = 7.0, CH_2O), 6.93 (2H, ddd, *J* = 1.9, *J* = 3.3, *J* = 8.8, Ar), 7.49 (2H, ddd, *J* = 1.8, *J* = 3.3, *J* = 8.8, Ar), 7.62 (2H, ddd, *J* = 1.8, *J* = 2.6, *J* = 8.8, Ar), 8.19 (2H, ddd, *J* = 1.8, *J* = 2.6, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 14.12, 22.54, 28.27, 28.99, 68.27, 115.20, 124.22, 127.09, 128.61, 130.87, 146.55, 147.36, 160.13

IR (v_{max} cm^{-1}): 532, 632, 694, 748, 825, 1010, 1111, 1188, 1249, 1334, 1396, 1465, 1504, 1597, 1720, 1921, 2322, 2870, 2931

MS m/z (mTOF, ESI+): 308.1241 ($C_{17}H_{19}NNaO_3$, M+Na), 286.1426 (100%, $C_{17}H_{20}NO_3$, M+H)

Assay (HPLC): 99.5%



4: 4-Hexyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl(1.0 g, 4.65 mmol), bromohexane (1.19 g, 1.01 ml 6.97 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 0.92 g (66%)

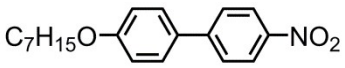
^{1}H NMR (400 MHz, $CDCl_3$): 0.83 (3H, t, *J* = 7.0, CH_3), 1.26 - 1.36 (4H, m, CH_2CH_2), 1.41 (2H, qnt, *J* = 7.0, CH_2), 1.74 (2H, qnt, *J* = 7.0, CH_2), 3.94 (2H, t, *J* = 7.0, CH_2O), 6.93 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.49 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.62 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar), 8.19 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 14.13, 22.69, 25.79, 29.26, 31.65, 68.29, 115.20, 124.23, 127.10, 128.61, 130.87, 146.55, 147.36, 160.13

IR (v_{max} cm^{-1}): 632, 694, 725, 756, 825, 995, 1026, 1103, 1172, 1242, 1334, 1388, 1473, 1512, 1597, 2862, 2931

MS m/z (mTOF, ESI+): 322.1397 ($C_{18}H_{22}NNaO_3$, M+Na), 300.1581 (100%, $C_{18}H_{22}NO_3$, M+H)

Assay (HPLC): 99.2%



5: 4-Heptyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl (1.0 g, 4.65 mmol), bromoheptane (1.29 g, 1.13 ml 6.97 mmol), potassium hydroxide (0.39 g, 6.97 mmol), ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 1.13 g (89%)

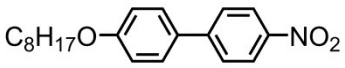
^{1}H NMR (400 MHz, $CDCl_3$): 0.88 (3H, t, *J* = 7.0, CH_3), 1.22 - 1.50 (8H, m, $CH_2CH_2CH_2CH_2$), 1.81 (2H, qnt, *J* = 7.0, CH_2), 4.00 (2H, t, *J* = 7.0, CH_2O), 6.89 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.54 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.66 (2H, ddd, *J* = 1.8, *J* = 2.6, *J* = 8.8, Ar), 8.24 (2H, ddd, *J* = 1.8, *J* = 2.6, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 14.18, 22.70, 26.08, 29.14, 29.30, 31.87, 68.29, 115.26, 124.22, 127.09, 128.61, 130.86, 146.55, 147.36, 160.13

IR (v_{max} cm^{-1}): 547, 609, 686, 756, 817, 848, 918, 1002, 1072, 1103, 1165, 1203, 1257, 1319, 1342, 1396, 1512, 1604, 1720, 2985

MS m/z (mTOF, ESI+): 336.1553 ($C_{19}H_{23}NNaO_3$, M+Na), 314.1740 (100%, $C_{19}H_{24}NO_3$, M+H)

Assay (HPLC) 99.2%



6: 4-Octyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl (500 mg, 2.325 mmol), bromooctane (897 mg, 0.8 ml 4.65 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 0.43 g (57%)

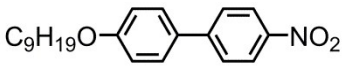
^{1}H NMR (400 MHz, $CDCl_3$): 0.87 (3H, t, *J* = 7.0, CH_3), 1.20 – 1.40 (8H, m, $CH_2CH_2CH_2CH_2$), 1.45 (2H, qnt, *J* = 7.0, CH_2), 1.79 (2H, qnt, *J* = 7.0, CH_2), 3.99 (2H, t, *J* = 7.0, CH_2O), 6.98 (2H, d, *J* = 8.8, Ar), 7.54 (2H, d, *J* = 8.8, Ar), 7.66 (2H, d, *J* = 8.8, Ar), 8.24 (2H, d, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 14.10, 22.64, 26.00, 29.18, 29.22, 29.33, 31.79, 68.16, 115.07, 124.11, 126.98, 128.49, 130.73, 146.40, 147.24, 160.00

IR (v_{max} cm^{-1}): 501, 632, 694, 717, 756, 825, 1033, 1111, 1188, 1249, 1334, 1465, 1504, 1597, 2322, 2854, 2916

MS m/z (mTOF, ESI+): 350.1718 ($C_{20}H_{25}NNaO_3$, M+Na), 328.1902 (100%, $C_{20}H_{26}NO_3$, M+H)

Assay (HPLC): 99.2%



7: 4-Nonyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl (500 mg, 2.325 mmol), bromononane (962.6 mg, 0.89 ml 4.65 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 650.7 mg (78%)

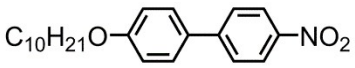
^{1}H NMR (400 MHz, $CDCl_3$): 0.87 (3H, t, *J* = 6.7, CH_3), 1.21 – 1.40 (10H, m, $CH_2CH_2CH_2CH_2CH_2$), 1.45 (2H, qnt, *J* = 6.7, CH_2), 1.79 (2H, qnt, *J* = 6.7, CH_2), 3.99 (2H, t, *J* = 6.7, CH_2O), 6.98 (2H, ddd, *J* = 2.1, *J* = 3.1, *J* = 8.9, Ar), 7.54 (2H, ddd, *J* = 2.1, *J* = 3.1, *J* = 8.9, Ar), 7.66 (2H, ddd, *J* = 1.8, *J* = 2.8, *J* = 8.9, Ar), 8.24 (2H, ddd, *J* = 1.8, *J* = 2.8, *J* = 8.9, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 14.09, 22.64, 25.99, 29.18, 29.24, 29.37, 29.50, 31.85, 68.16, 115.08, 124.09, 126.95, 128.47, 130.71, 146.40, 147.22, 160.01

IR (v_{max} cm^{-1}): 524, 632, 694, 717, 756, 825, 856, 979, 1010, 1033, 1111, 1188, 1249, 1303, 1334, 1396, 1465, 1504, 1597, 2846, 2916, 3070

MS m/z (mTOF, ESI+): 364.1869 ($C_{21}H_{27}NNaO_3$, M+Na), 342.2052 (100%, $C_{21}H_{28}NO_3$, M+H)

Assay (HPLC): 99.3%



8: 4-Decyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl(500 mg, 2.325 mmol), bromodecane (1.03 g, 0.96 ml 4.65 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 0.43 g (52%)

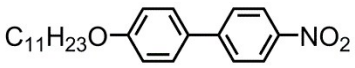
^{1}H NMR (400 MHz, $CDCl_3$): 0.86 (3H, t, *J* = 7.0, CH_3), 1.20 – 1.40 (12H, m, $CH_2CH_2CH_2CH_2CH_2CH_2$), 1.44 (2H, qnt, *J* = 7.0, CH_2), 1.79 (2H, qnt, *J* = 7.0, CH_2), 3.99 (2H, t, *J* = 7.0, CH_2O), 6.98 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.54 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.66 (2H, ddd, *J* = 1.8, *J* = 2.6, *J* = 8.8, Ar), 8.24 (2H, ddd, *J* = 1.8, *J* = 2.6, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 14.10, 22.66, 25.99, 29.17, 29.30, 29.36, 29.53, 29.55, 31.87, 68.15, 115.07, 124.10, 126.96, 128.48, 130.71, 146.40, 147.23, 160.00

IR (v_{max} cm^{-1}): 540, 632, 694, 725, 756, 825, 856, 1026, 1111, 1180, 1249, 1334, 1465, 1504, 1597, 2322, 2854, 2924

MS m/z (mTOF, ESI+): 378.2021 ($C_{22}H_{29}NNaO_3$, M+Na), 356.2205 (100%, $C_{22}H_{30}NO_3$, M+H)

Assay (HPLC): 99.5%



9: 4-Undecyloxy-4'-nitrobiphenyl

Quantities used: 4-Hydroxy-4′-nitrobiphenyl(500 mg, 2.325 mmol), bromoundecane (1.09 g, 1.04 ml 4.65 mmol), potassium hydroxide (0.39 g, 6.97 mmol) and ethanol (50 ml). The general experimental procedure was followed; recrystalisation from hexane afforded the title compound as pale yellow needles.

Yield: 0.5 g (58%)

^{1}H NMR (400 MHz, $CDCl_3$): 0.86 (3H, t, *J* = 7.0, CH_3), 1.19 – 1.40 (14H, m, $CH_2CH_2CH_2CH_2CH_2CH_2CH_2$), 1.43 (2H, qnt, *J* = 7.0, CH_2), 1.79 (2H, qnt, *J* = 7.0, CH_2), 3.99 (2H, t, *J* = 7.0, CH_2O), 6.98 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.54 (2H, ddd, *J* = 1.8, *J* = 3.0, *J* = 8.8, Ar), 7.66 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar), 8.24 (2H, ddd, *J* = 2.2, *J* = 2.6, *J* = 8.8, Ar)

^{13}C NMR (100.5 MHz, $CDCl_3$): 14.11, 22.67, 25.99, 29.18, 29.32, 29.37, 29.55, 29.58, 31.89, 68.16, 115.08, 124.10, 126.97, 128.48, 130.73, 146.41, 147.24, 160.00

IR (v_{max} cm^{-1}): 547, 632, 694, 717, 756, 825, 856, 1010, 1033, 1103, 1103, 1180, 1242, 1303, 1334, 1396, 1473, 1512, 1597, 2846, 2916

MS m/z (mTOF, ESI+): 392.2170 ($C_{23}H_{31}NNaO_3$, M+Na), 370.2359 (100%, $C_{23}H_{32}NO_3$, M+H)

Assay (HPLC): 99.7%

1.4. Supplemental SAXS Data

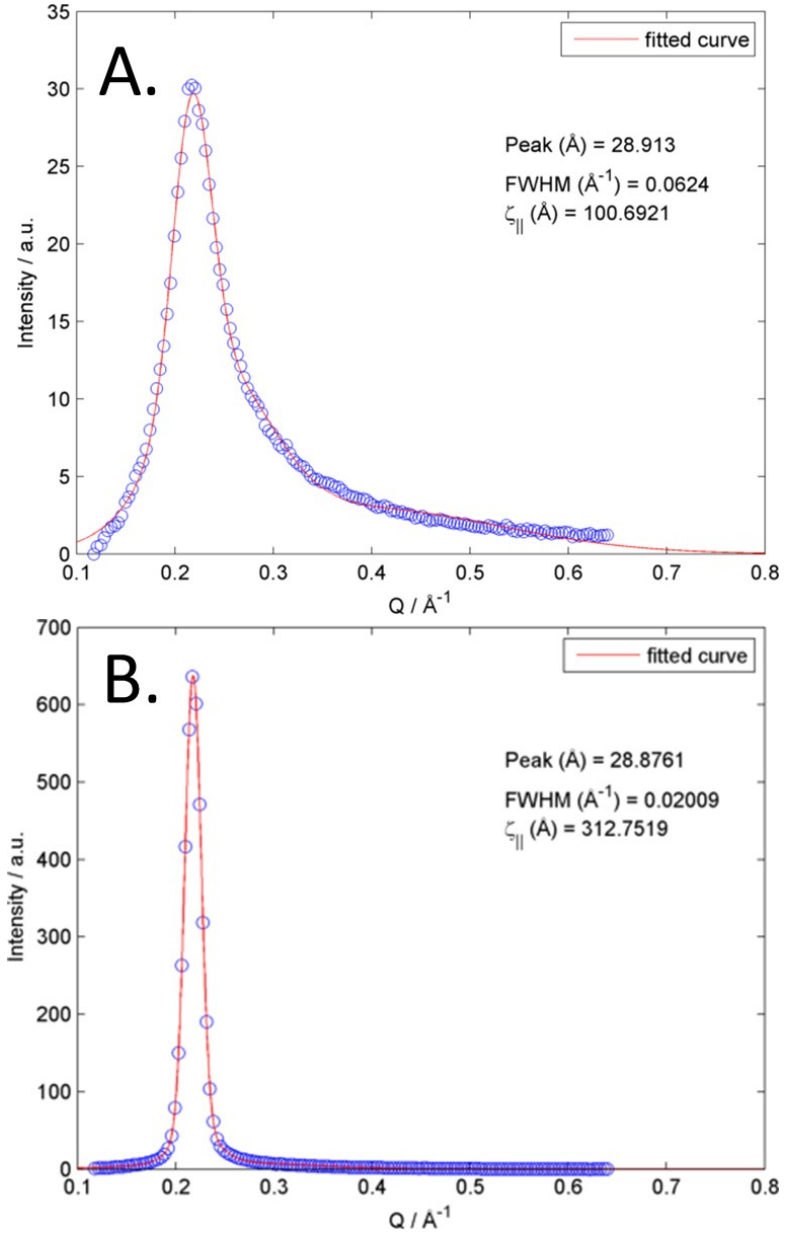


Figure SI-1: Examples of fitted data used to obtain d-spacings for small angle scattering peaks: (A) the nematic phase of compound **6** at 51 °C; (B) the smectic A_D phase of compound **6** at 46 °C. Blue circles correspond to SAXS data while the solid red line is a 3-term Gaussian function fitted to the raw data. The R^2 values of the fits are 0.99678 and 0.99992 for A and B respectively.

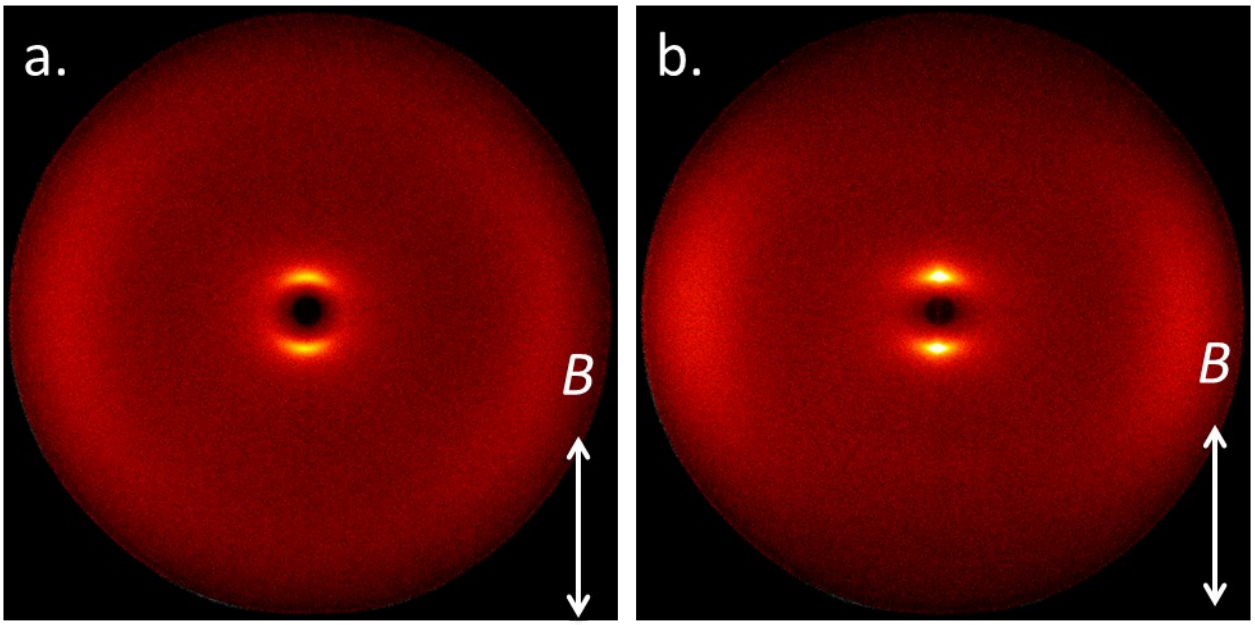


Figure SI-2: Magnetically aligned 2D SAXS patterns for compound **6** in the nematic phase at 51 °C (a) and in the smectic A phase at 45 °C (b).

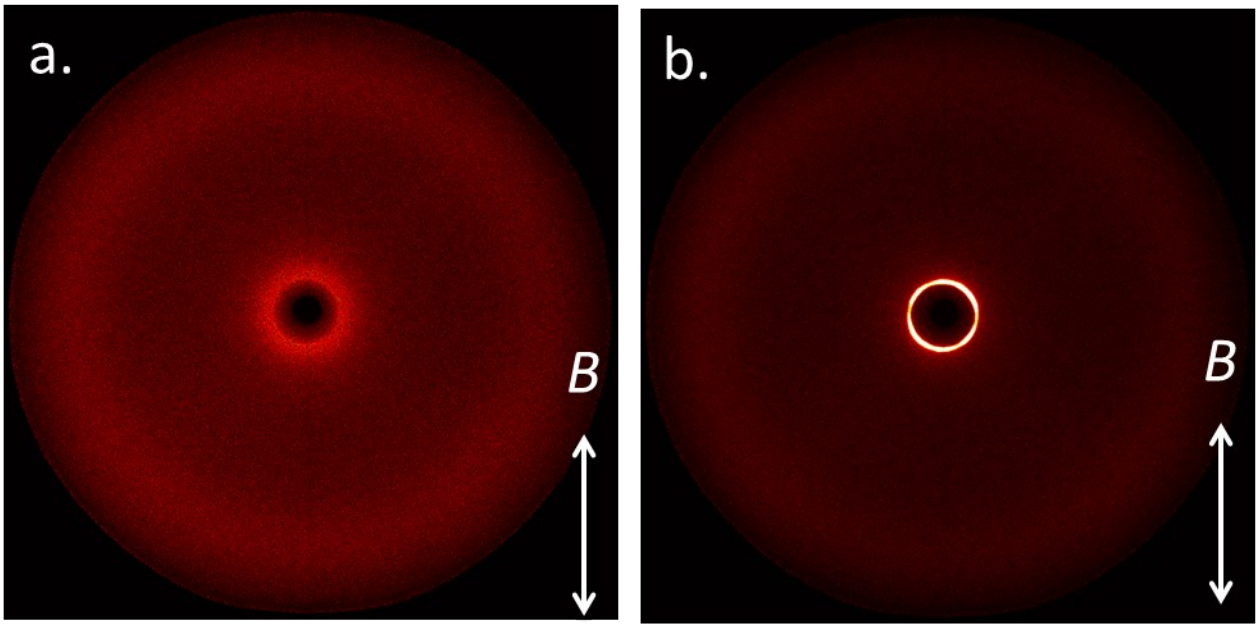


Figure SI-3: Unaligned 2D SAXS patterns for compound **7** in the isotropic liquid at 54 °C (a) and in the smectic A phase at 44 °C (b).

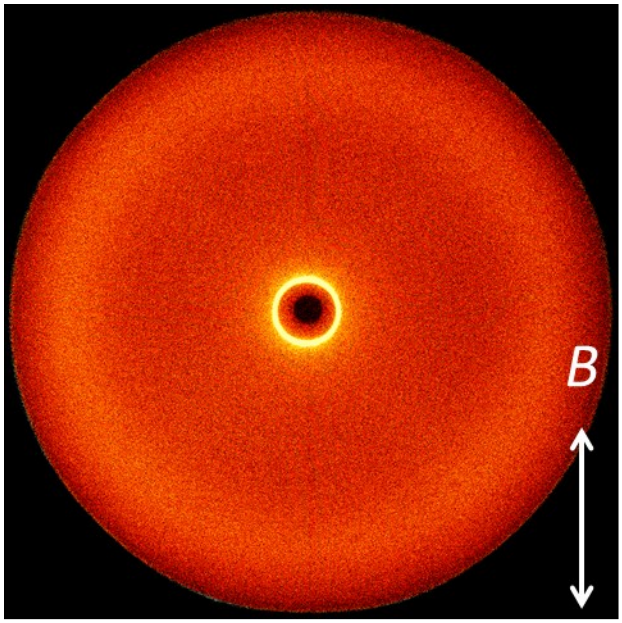


Figure SI-4: Unaligned 2D SAXS patterns for compound **8** in the smectic A phase at 55 °C. The sample could not be aligned by the applied magnetic field.

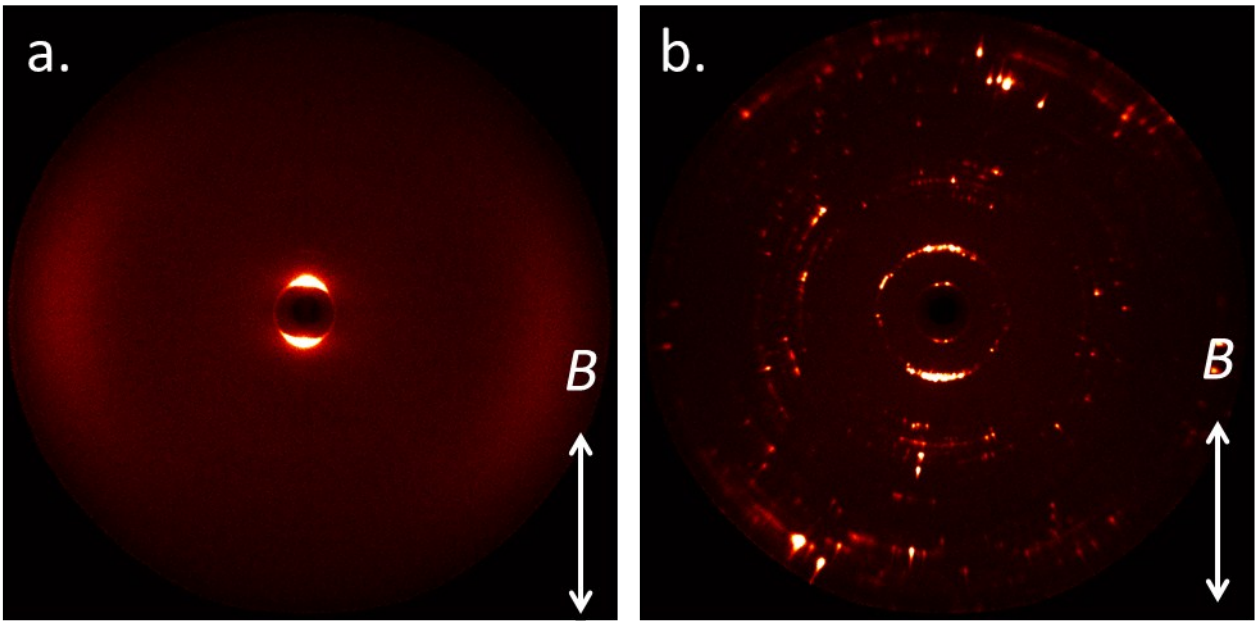


Figure SI-5: (a) Partially magnetically aligned 2D SAXS pattern for the SmA phase of compound **9** at 52 °C, (b) 2D SAXS pattern of compound **9** following recrystalisation at 35 °C

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