

***Supporting Information***

**Shape-persistent V-Shaped Mesogens –Formation of Nematic  
Phases with Biaxial Order**

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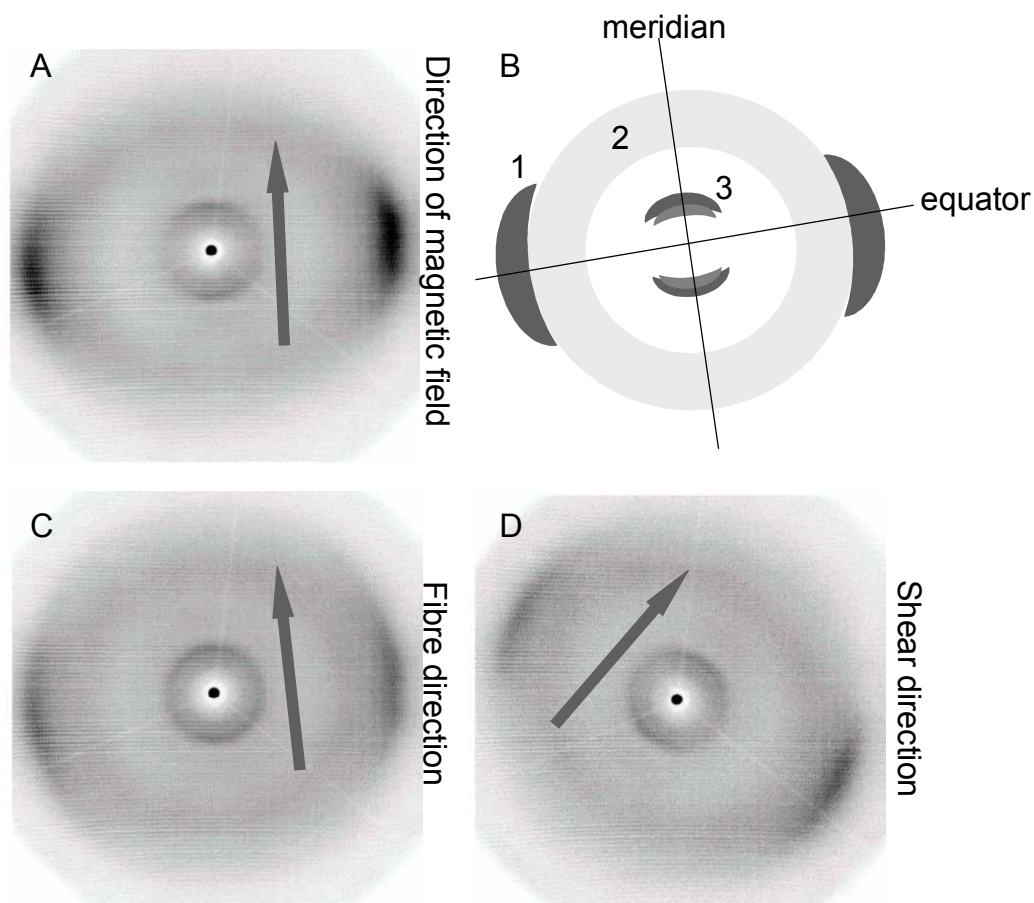
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**TABLE S1:** Comparison of  $^{13}\text{C}$  data of molecules **1a-c**.

Compounds	OCH <sub>2</sub>	C (C≡C)	CH <sub>aromat</sub>	C <sub>q,aromat</sub> , CN, CO
<b>1a</b>	69.6 69.7	85.8 90.1 94.3 95.3	116.8, 117.0, 123.1, 124.3, 128.3, 128.4, 131.6, 132.7	113.0, 115.0, 123.3, 130.0, 133.6, 143.7, 153.6, 153.9, 191.9
<b>1b</b>	69.5 69.6	89.7 90.3 93.4 94.7	116.7, 123.1, 124.3, 131.96, 132.0, 132.7	111.5, 113.6, 114.1, 118.5, 128.2, 129.8, 133.7, 143.7, 153.8, 153.9, 191.8
<b>1c</b>	69.6 69.7 69.5	85.5 90.1 94.3 95.3 89.7 90.4 93.4 94.7	116.8, 117.0, 123.1, 124.3, 128.3, 128.4, 131.6, 131.9, 132.0, 132.7	111.4, 112.9, 113.5, 114.1, 115.0, 118.5, 123.3, 129.8, 130.0, 133.5, 133.7, 143.66, 143.71, 153.6, 153.8, 153.9, 191.8

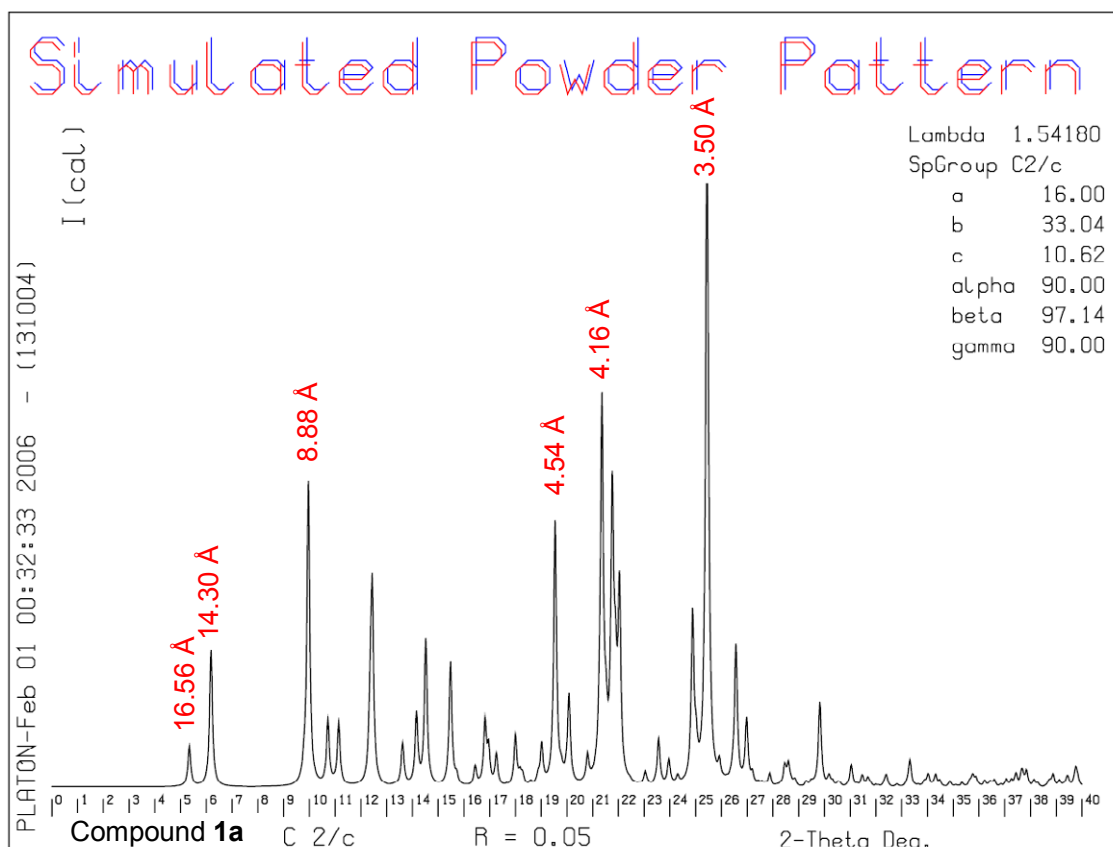
NMR data of compound **1c** consists of both signal sets observed for the symmetric molecules **1a** and **1b**.

**Figure S1:** X-ray of differently aligned samples **1b** at 30 °C.



**A:** Alignment by fast cooling in a strong magnetic field (7T); **B:** Schematic representation with (1) the halo attributed to the  $\pi$ - $\pi$  interaction of aromatic units, (2) the halo related to the mean distance of aliphatic chains and (3) the reflection arcs associated with the distances along the bisect of the molecules. **C:** X-ray pattern from a drawn fibre; **D:** X-ray pattern from a shear aligned sample.

**Figure S2:** Simulated powder diffraction pattern obtained from the crystal structure of **1a**.



In the wide angle region of the powder pattern of sample **1a** (Figure 2) the strongest reflections (e.g. (312) = 3.50 Å and (202) = 4.16 Å) originate from alkyl chains, which appear only as a broad halo at approx. 4.5 Å in the LC phase. The third strongest peak ((021) and (02-1) = 8.86 Å) represents the mean distance of phenylene ethynylene arms and is not available in the powder pattern of **1b** and **1c** in their nematic phases. Two weaker reflections ((020) = 16.56 Å and (110) = 14.30 Å) arise in the low angle region. Both are related with the distances between the fluorenone stacks viewed along the *c*-axis and are reminiscent of the molecular dimensions along the bisect of the V-shaped molecules. As outlined in the article, the correlation lengths are about two molecules most likely along the **l** director in the nematic phase. Thus high order reflections and reflections with mixed indices will presumably not result in visible signals. However, the single crystal of **1a** show possible arrangements and distances for these molecules, which can help to generate a model for the orientation of V-shaped mesogens in their biaxial liquid crystal structure (cf. Figure 3, see below).

**Figure S3:** View along the *c*-axis of the single crystal structure of **1a**. Distances between 2,5-alkoxy substituted benzene units are shown which are comparable to *d*-values found for nematic phases at small angles (e.g. 21.6 Å and 14.5 Å for **1c**).

