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Supporting information for article:

Crystal and mesophase structure of a bicyclohexyl cyano mesogen

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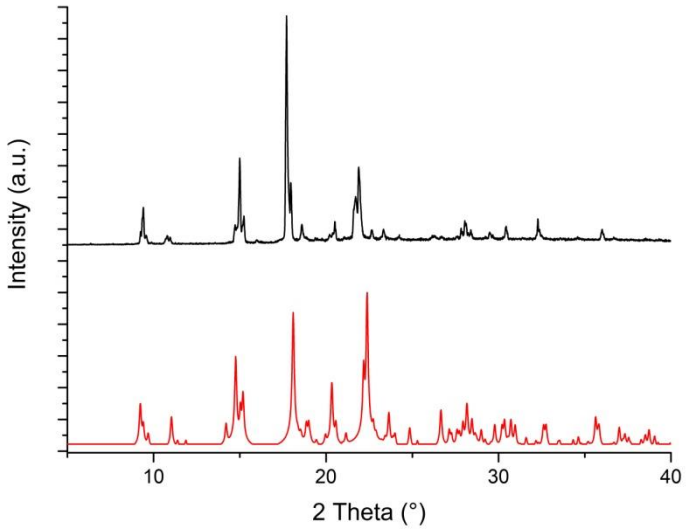

Fig. S1. Comparison between the X-ray powder patterns calculated from single crystal analysis (red line) and measured on the crystalline powder (black line) of the title compound

We have found for the S_E phase of **1** a strong tendency to preferential alignment for samples obtained after melting of the crystalline powder. In fact, the X-ray diffraction pattern recorded at 95 °C from the LC phase obtained upon melting of the crystalline sample, only shows the wide-angle halo, without the low and medium angle reflections, and this pattern persists up to the isotropization, Fig. S2. Instead, for the mesophase obtained by cooling the isotropic liquid, the diffraction pattern of Fig. 7 of the typescript is obtained.

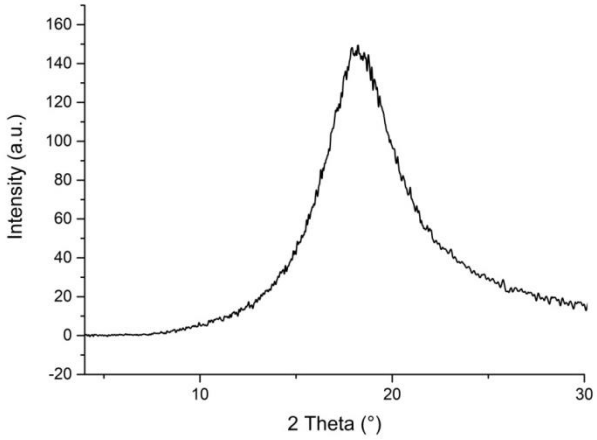

Fig. S2. PXRD pattern of the sample at 95°C (heating cycle).

In recording the diffraction pattern from the LC phase, the sample was put on a Si substrate. We have performed a different experiment, in which the sample was put on a glass substrate and this, in turn, was put on the Si plate for recording the diffraction pattern. In this case, the diffraction pattern recorded for the LC phase, also on heating, is basically like the pattern of Fig. 7 of the typescript, and this confirms the hypothesis of preferential alignment. The type of alignment leading to the diffraction pattern of Fig. S2 can be understood with reference to Fig. S3.

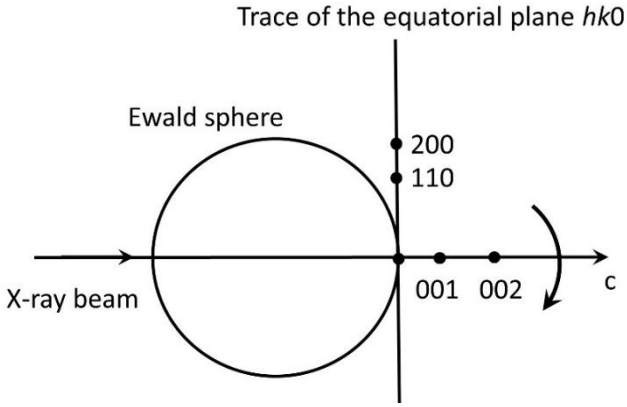

Fig. S3. Alignment of the LC phase.

We can suppose that the smectic layers are oriented perpendicular to the direction of the incident X-rays, and so the *c* axis is parallel to the X-ray beam, Fig. S3. In this case, even assuming full rotational disorder around *c* axis, the meridional (reciprocal) lattice points 001, 002, and the equatorial lattice points 110 and 200 never intersect the Ewald sphere, and so they do not produce diffracted beams.