Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

An insight into de Vries behaviour of smectic liquid crystals from atomistic molecular dynamics simulations

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DFT optimised 9HL structures and energies

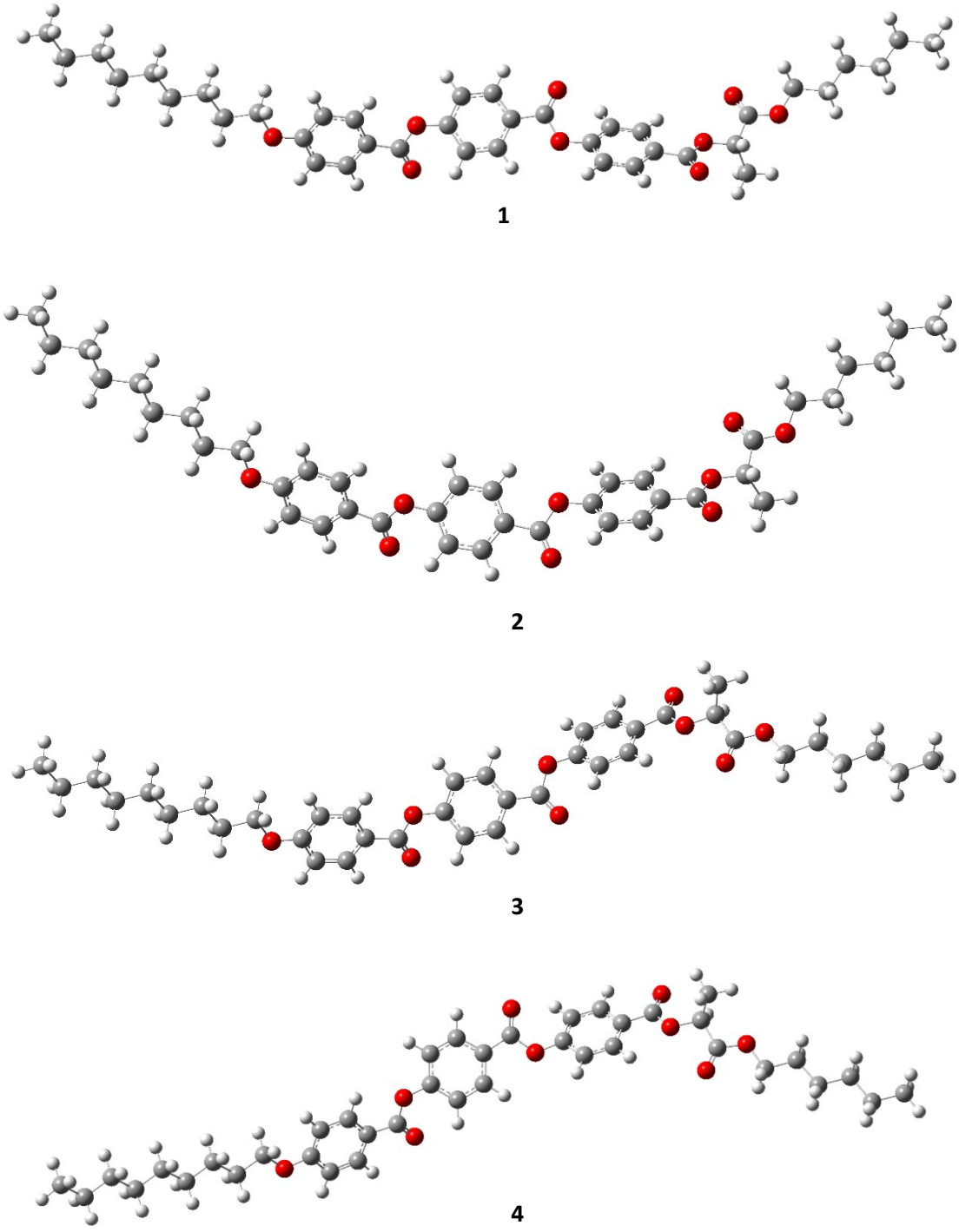


Figure S1 The four optimised conformers of 9HL, calculated at the B3LYP/6-31G(d) level

Table S1 Energies of the four 9HL conformers calculated at the B3LYP/6-31G(d) level

Conformer	E / Ha	ΔE / kJ mol^{-1}
1	-2192.16583195	0.416
2	-2192.16586777	0.322
3	-2192.16569003	0.789
4	-2192.16599035	0.000

R values from reported tilt angles and layer spacings

As stated in the main text, *R* values derived from reported experimental investigations of 9HL have significant uncertainty associated with them. This is due to the range of layer spacings and tilt angles reported for 9HL, combined with the variation of *R* with temperature. Figure S2 below shows the variation in *R* values with temperature, using layer spacings and tilt angles from a range of experimental reports.[S1-S4]

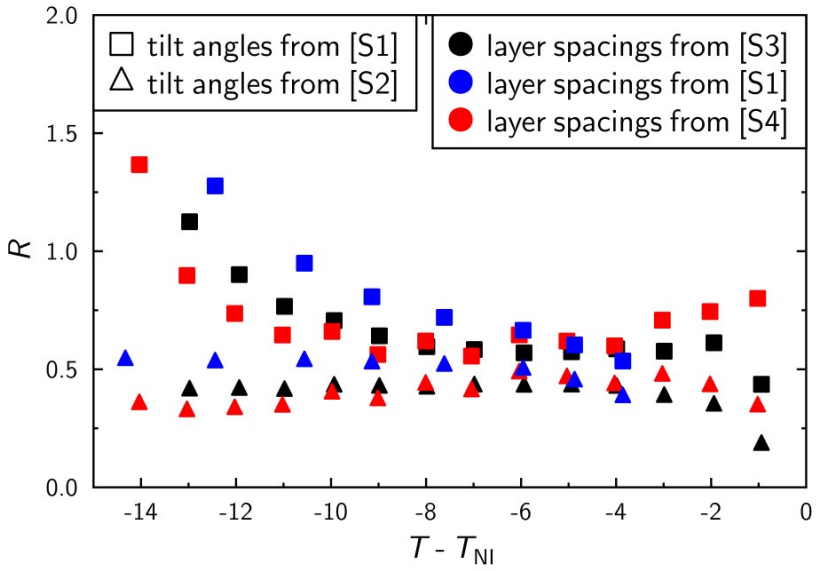
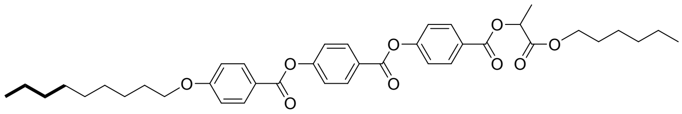


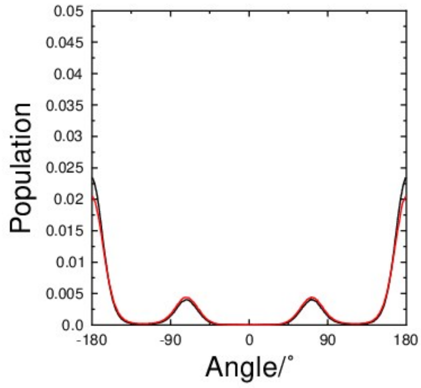
Figure S2 *R* values determined from reported experimental tilt angles and layer spacings of 9HL. Marker shapes indicate the reported tilt angles used and marker colours indicate the reported layer spacings used.

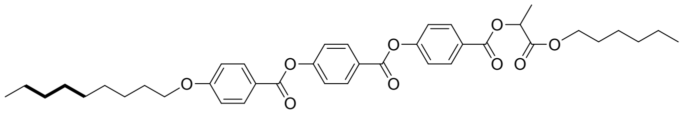
Table S1 Order parameters P_2, P_4, P_6 and P_8, determined with respect to **k**, obtained from from orientational distribution functions of the minimum MOI axes of 9HL at 10 K intervals between 330 K and 400 K (Figure 7 of the main text).

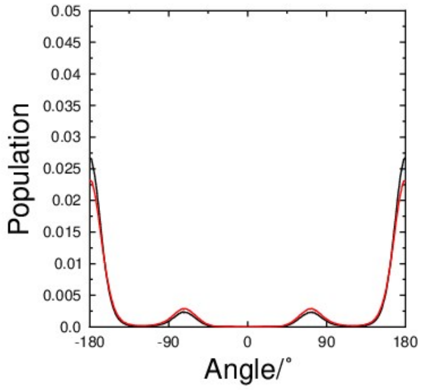
T / K	P_2	P_4	P_6	P_8
330	0.751	0.378	0.099	-0.020
340	0.767	0.399	0.094	-0.050
350	0.773	0.424	0.135	-0.008
360	0.838	0.578	0.326	0.152
370	0.838	0.588	0.338	0.161
380	0.837	0.578	0.326	0.153
390	0.812	0.545	0.296	0.133
400	0.799	0.523	0.274	0.118

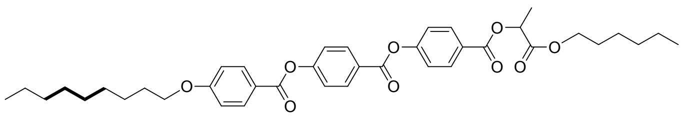
Dihedral populations from simulations at 340 K (SmC*) and at 380 K (SmA*)

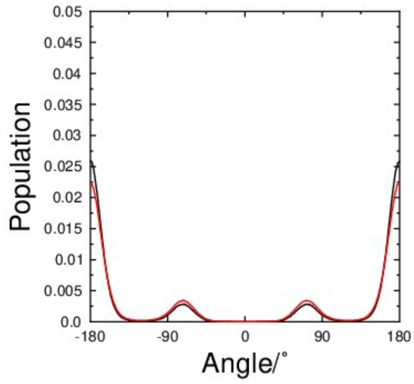


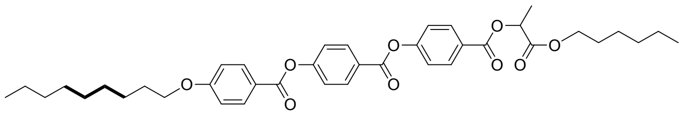


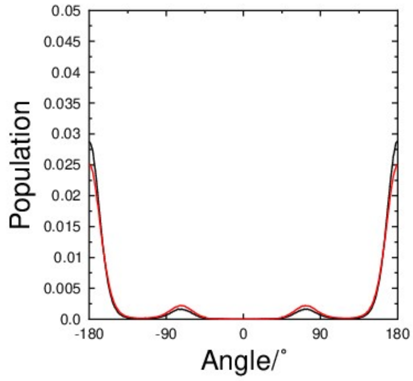


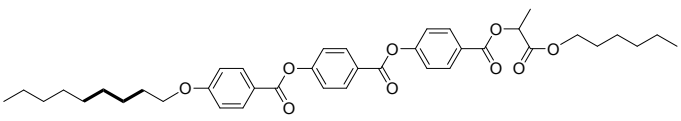


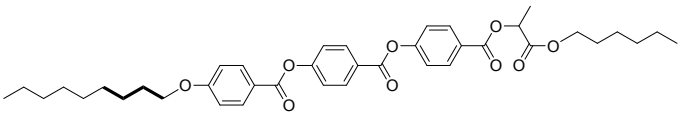


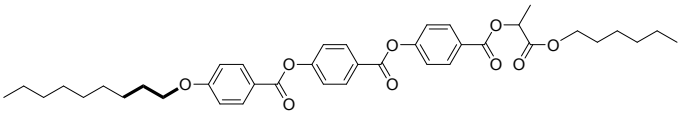


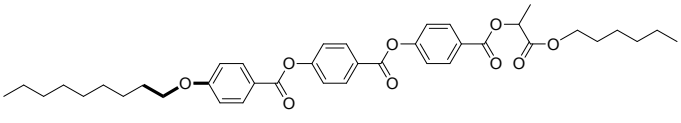


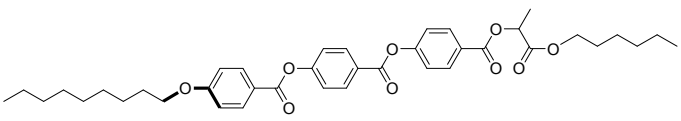


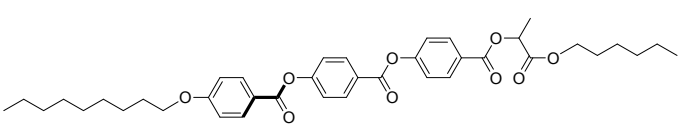


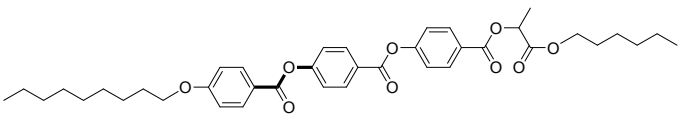


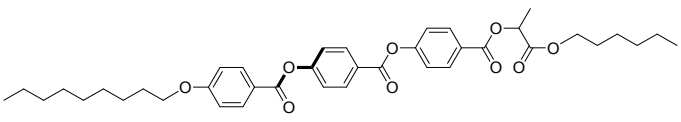


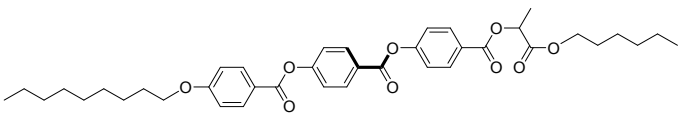


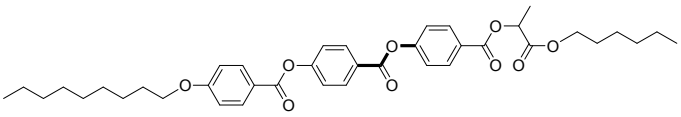


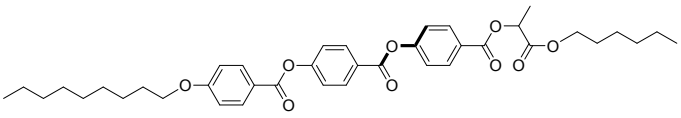


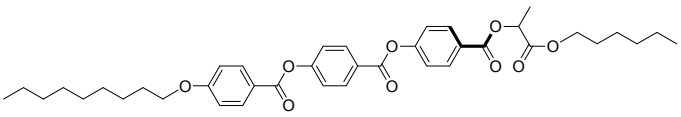


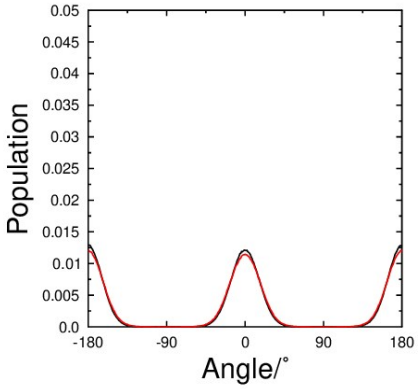








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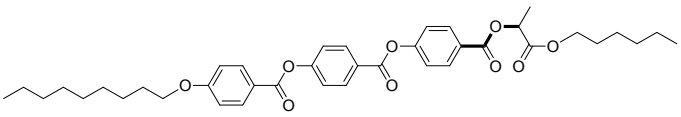

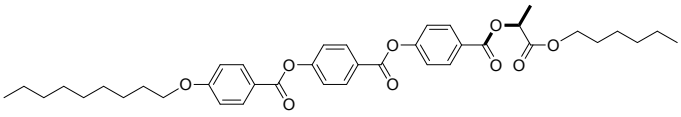

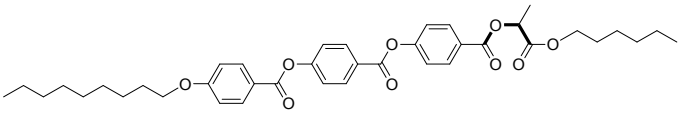

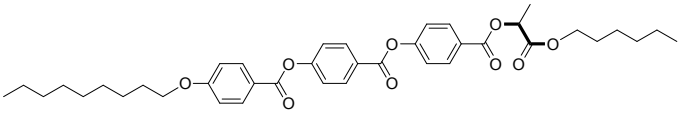

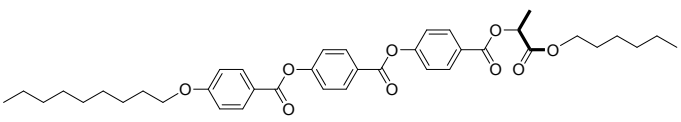

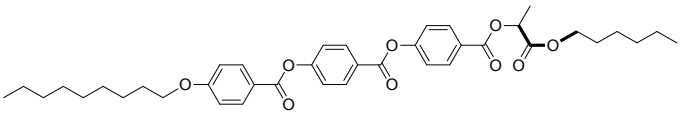

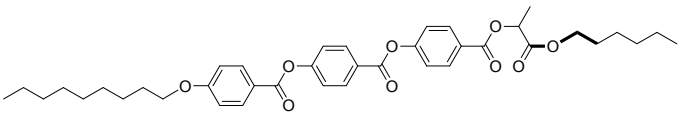

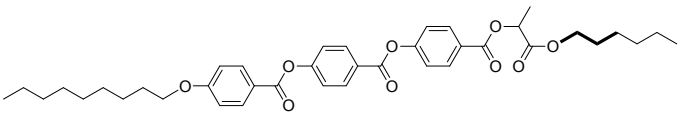

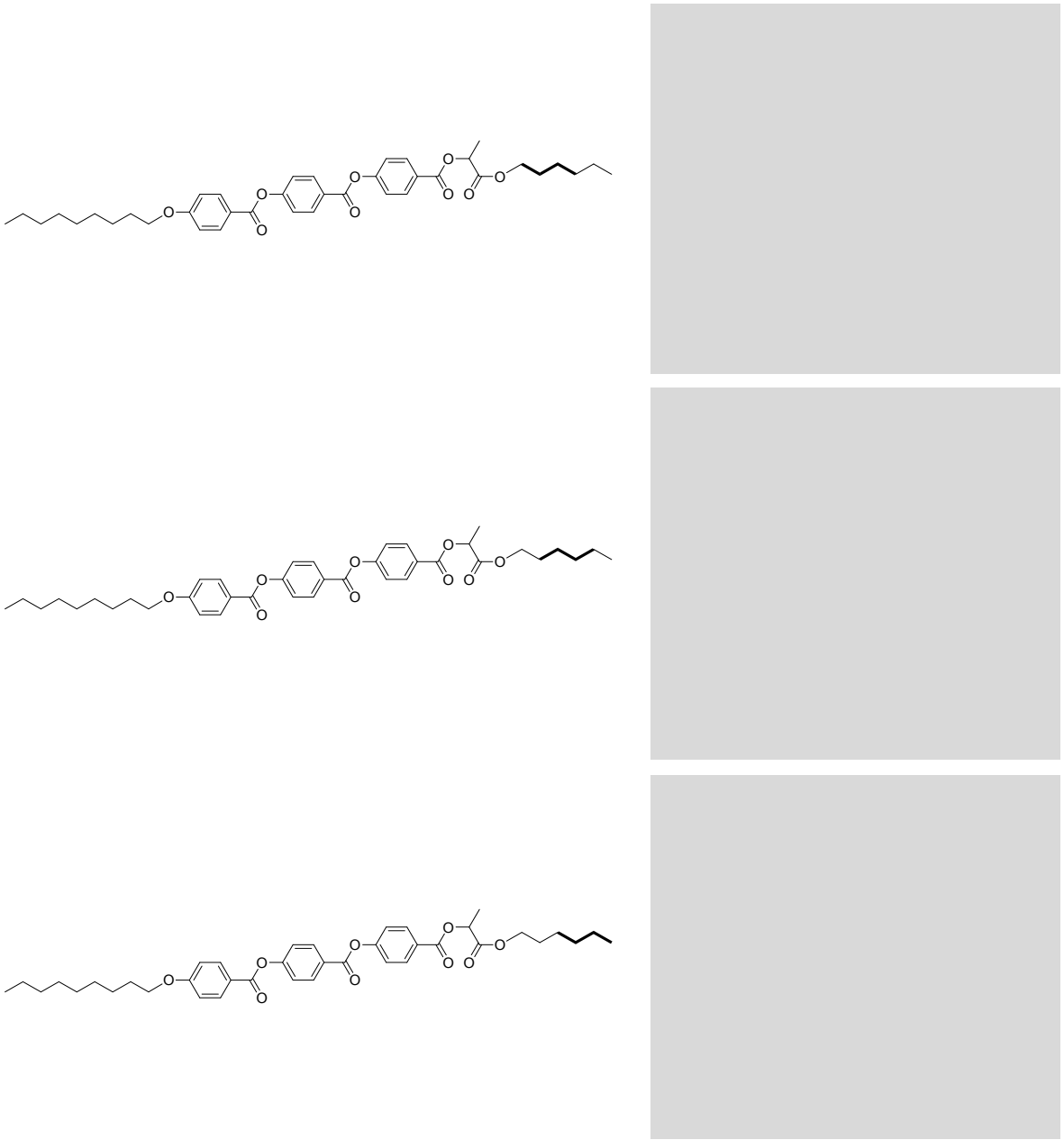

Figure S3 Populations of dihedral angles (shown in bold) in 9HL at 340 K (SmC*; black) and at 380 K (SmA*; red).

References

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