Electronic Supplementary Information

New bent-core mesogens with carbon-carbon multiple linkages in the terminal chains

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Analytical data:

Analytical data are given for the compounds A16/in-11 and B14/in-3 as representatives for members of series A and B:

Bis[4-(4-n-hexadec-11-inyloxycarbonylbenzylideneamino)phenyl] isophthalate (A16/in-11)

Melting behaviour: see Table 1
Elemental analysis: C_{68}H_{80}O_{8}N_{2} (Mm = 1053.34); C 77.53, H 7.66, N 2.66 (calc.); C 77.18, H 7.83, N 2.31 (found);
{[^1]}H-NMR (400 MHz, CDCl₃): δ 0.88 (m, 6H, CH₃), 1.29-1.52 (m, 36H, CH₂), 1.78 (m, 4H, ArCOOCH₂CH₂C≡CCH₂), 2.12 (m, 8H, CH₂C≡CCH₂), 4.33 (t, J = 6.7 Hz, 4H, ArCOOCH₂CH₂), 7.30 (m, 8H, Ar-H), 7.69 (t, J = 7.9 Hz, 1H, Ar-H), 7.97 (d, J = 8.5 Hz, 4H, Ar-H), 8.13 (d, J = 8.5 Hz, 4H, Ar-H), 8.47 (m, 2H, Ar-H), 8.53 (s, 2H, CH=N), 9.03 (s, 1H, Ar-H).

Bis[4-(4-n-tetradec-3-inyloxycarbonyl)ethenylbenzylideneamino]phenyl] isophthalate (B14/in-3)

Melting behaviour: see Table 2
Elemental analysis: C_{68}H_{76}O_{8}N_{2} (Mm = 1049.31): C 77.83, H 7.30, N 2.67 (calc.); C 77.54, H 7.45, N 2.40 (found);
{[^1]}H-NMR (400 MHz, CDCl₃): δ 0.86 (t, J = 6.9 Hz, 6H, CH₃), 1.23-1.51 (m, 32H, CH₂), 2.14 (m, 4H, ArCH=CHCOOCH₂CH₂C≡CCH₂), 2.56 (m, 4H, ArCH=CHCOOCH₂CH₂C≡CCH₂), 6.52 (d, J = 16.0 Hz, 2H, ArCH=CHCOOCH₂CH₂C≡CCH₂), 7.30 (m, 8H, Ar-H), 7.69 (t, J = 7.5 Hz, 1H, Ar-H), 7.72 (d, J = 16.0 Hz, 2H, ArCH=CHCOOCH₂), 7.92 (d, J = 8.3 Hz, 4H, Ar-H), 8.47 (m, 2H, Ar-H), 8.48 (s, 2H, CH=N), 9.02 (s, 1H, Ar-H).
Table S1: References of bent-core mesogens containing different unsaturated chains R at one or both terminal positions (R is related to the general formula shown in Scheme 1)

![Scheme 1](image)

<table>
<thead>
<tr>
<th>-R</th>
<th>n</th>
<th>R at one terminal position</th>
<th>R at both terminal positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>-O-(CH$_2$)$_n$-CH=CH$_2$</td>
<td>9, 8</td>
<td>[S1-S7]</td>
<td>[S6, S10-S14]</td>
</tr>
<tr>
<td>-COO-(CH$_2$)$_n$-CH=CH$_2$</td>
<td>8</td>
<td></td>
<td>[S12]</td>
</tr>
<tr>
<td>-O-(CH$<em>2$)$</em>{10}$CH=CHCH$_3$ (cis)</td>
<td></td>
<td></td>
<td>[S15]</td>
</tr>
<tr>
<td>-O-(CH$_2$)$_n$CH=CHC$<em>8$H$</em>{17}$ (cis)</td>
<td></td>
<td></td>
<td>[S15]</td>
</tr>
<tr>
<td>-O-(CH$_2$)$_n$OOCCH=CH$_2$</td>
<td>11,12</td>
<td>[S8]</td>
<td>[S15-S17]</td>
</tr>
<tr>
<td>-O-(CH$_2$)$_n$OOCC(CH$_3$)=CH$_2$</td>
<td>6,11,12</td>
<td>[S8]</td>
<td>[S15-S16]</td>
</tr>
<tr>
<td>-O-(CH$_2$)$_n$CH=CH-CH=CH$_2$</td>
<td>8, 10, 14</td>
<td></td>
<td>[S18]</td>
</tr>
<tr>
<td>-O-(CH$_2$)$_n$OCH$_2$CH=CH$_2$</td>
<td></td>
<td></td>
<td>[S9]</td>
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</table>
Table S 2: Effect of the insertion of C=C bonds into both terminal chains on the mesophase behaviour of bent-core mesogens with increasing aromatic core. ΔT means the depression of the clearing temperatures caused by replacement the undecyloxy with undecenyloxy chains.

![Central unit structure](image)

<table>
<thead>
<tr>
<th>Central unit</th>
<th>R-</th>
<th>Mesophase behaviour</th>
<th>ΔT</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Central unit structure" /></td>
<td>C_{11}H_{23}O-</td>
<td>Cr 105 SmCP_A 113 I [S10]</td>
<td></td>
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<tr>
<td></td>
<td>CH_2=CH-C_{9}H_{18}O-</td>
<td>Cr 101 SmCP_A 95 I [S11]</td>
<td>ΔT = -18K</td>
</tr>
<tr>
<td><img src="image" alt="Central unit structure" /></td>
<td>C_{11}H_{23}O-</td>
<td>Cr 85 N 113 I [S19]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CH_2=CH-C_{9}H_{18}O-</td>
<td>Cr 79 N 83 I [S11]</td>
<td>ΔT = -20K</td>
</tr>
<tr>
<td><img src="image" alt="Central unit structure" /></td>
<td>C_{11}H_{23}O-</td>
<td>Cr 136 SmCP_A 169 I [S20]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CH_2=CH-C_{9}H_{18}O-</td>
<td>Cr 126 SmCP_A 158 I [S12]</td>
<td>ΔT = -11K</td>
</tr>
<tr>
<td><img src="image" alt="Central unit structure" /></td>
<td>C_{11}H_{23}O-</td>
<td>Cr 87 Col_r 157 I [S21]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CH_2=CH-C_{9}H_{18}O-</td>
<td>Cr 99 Col_r 146 I [S10]</td>
<td>ΔT = -11K</td>
</tr>
</tbody>
</table>
Figs. S1 – S6: POM images of compound A14/in-3 for further studies of the growing process of spiral filaments of different shape, myelinic-like and banana leaf-like domains, ribbon-like or circular domains, which can simultaneously occur in the same sample (thickness 6 µm and 10 µm) on slow cooling the isotropic liquid.
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References in ESI: