Supplemental Material

Prediction of clearing temperatures of bent-core liquid crystals using decision trees and multivariate adaptive regression splines

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Table S1. Molecular structure of bent-core liquid crystals and their clearing temperatures

| Comp. | Molecular structure | Obs. temp. (K) | Ref. |
|-------|---------------------|----------------|------|
| 1     | R = C₆H₁₃           | 453.35         | [1]  |
| 2     | R = C₈H₁₇           | 449.05         | [1]  |
| 3*    | R = C₁₀H₂₁          | 444.45         | [1]  |
| 4     | R = C₁₂H₂₅          | 440.85         | [1]  |
| 5     | R = C₄H₉            | 409.25         | [2]  |
| 6*    | R = C₅H₁₁           | 408.05         | [2]  |
| 7     | R = C₆H₁₃           | 409.95         | [2]  |
| 8     | R = C₇H₁₅           | 407.85         | [2]  |
| 9     | R = C₈H₁₇           | 407.55         | [2]  |
| 10    | R = C₉H₁₉           | 408.75         | [2]  |
| 11    | R = C₁₀H₂₁          | 410.55         | [2]  |
| 12    | R = C₁₁H₂₃          | 410.75         | [2]  |
| 13    | R = C₁₂H₂₅          | 412.05         | [2]  |
| 14    | R = C₁₄H₂₉          | 411.45         | [2]  |
| 15    | R = C₁₆H₃₃          | 410.95         | [2]  |
| 16    | R = C₄H₉            | 445.35         | [2]  |
| 17    | R = C₃H₁₁           | 425.15         | [2]  |
| 18    | R = C₆H₁₃           | 428.15         | [2]  |
| 19    | R = C₇H₁₅           | 429.95         | [2]  |
| 20    | R = C₈H₁₇           | 435.05         | [2]  |
| 21    | R = C₉H₁₉           | 436.15         | [2]  |
| 22    | R = C₁₀H₂₁          | 439.55         | [2]  |
| 23    | R = C₁₁H₂₃          | 441.35         | [2]  |
| 24    | R = C₁₂H₂₅          | 444.75         | [2]  |
|   | Chemical Structure | R = C_nH_{2n+1} |     |     |
|---|-------------------|------------------|-----|-----|
| 25 | ![Chemical Structure](image1.png) | C_{10}H_{19} | 415.35 | [2] |
| 26 | ![Chemical Structure](image2.png) | C_{10}H_{21} | 415.25 | [2] |
| 27 | ![Chemical Structure](image3.png) | C_{11}H_{23} | 413.15 | [2] |
| 28 | ![Chemical Structure](image4.png) | C_{12}H_{25} | 412.85 | [2] |
| 29 | ![Chemical Structure](image5.png) | C_{8}H_{13} | 436.05 | [2] |
| 30 | ![Chemical Structure](image6.png) | C_{8}H_{15} | 434.85 | [2] |
| 31*| ![Chemical Structure](image7.png) | C_{8}H_{17} | 438.55 | [2] |
| 32 | ![Chemical Structure](image8.png) | C_{10}H_{19} | 436.25 | [2] |
| 33 | ![Chemical Structure](image9.png) | C_{10}H_{21} | 435.75 | [2] |
| 34 | ![Chemical Structure](image10.png) | C_{11}H_{23} | 433.55 | [2] |
| 35 | ![Chemical Structure](image11.png) | C_{12}H_{25} | 433.35 | [2] |
| 36 | ![Chemical Structure](image12.png) | C_{14}H_{29} | 432.15 | [2] |
| 37 | ![Chemical Structure](image13.png) | C_{16}H_{33} | 428.35 | [2] |
| 38 | ![Chemical Structure](image14.png) | C_{4}H_{9} | 414.95 | [2] |
| 39*| ![Chemical Structure](image15.png) | C_{6}H_{13} | 415.85 | [2] |
| 40*| ![Chemical Structure](image16.png) | C_{8}H_{17} | 408.25 | [2] |
| 41 | ![Chemical Structure](image17.png) | C_{10}H_{21} | 410.55 | [2] |
| 42*| ![Chemical Structure](image18.png) | C_{12}H_{25} | 410.75 | [2] |
| 43 | ![Chemical Structure](image19.png) | C_{14}H_{29} | 406.55 | [2] |
| 44 | ![Chemical Structure](image20.png) | C_{16}H_{33} | 405.45 | [2] |
| 45 | ![Chemical Structure](image21.png) | C_{18}H_{37} | 398.55 | [2] |
|   | ![Structure](image1) |   |
|---|---------------------|---|
|46 | \( R = \text{C}_6\text{H}_{13} \) | 432.75 [3] |
|47 | \( R = \text{C}_8\text{H}_{17} \) | 428.65 [3] |
|48 | \( R = \text{C}_{10}\text{H}_{21} \) | 422.65 [3] |
|49 | \( R = \text{C}_{12}\text{H}_{25} \) | 417.95 [3] |
|50*| \( R = \text{C}_6\text{H}_{13} \) | 404.15 [4] |
|51*| \( R = \text{C}_8\text{H}_{17} \) | 384.15 [4] |
|52 | \( R = \text{C}_9\text{H}_{19} \) | 383.15 [4] |
|53 | \( R = \text{C}_{10}\text{H}_{21} \) | 380.15 [4] |
|54 | \( R = \text{C}_{12}\text{H}_{25} \) | 382.15 [4] |
|55 | \( R = \text{C}_{14}\text{H}_{29} \) | 374.15 [4] |
|56 | \( R = \text{C}_{16}\text{H}_{33} \) | 375.15 [4] |
|57*| \( R = \text{C}_{18}\text{H}_{37} \) | 376.15 [4] |
|58 | \( R = \text{C}_{20}\text{H}_{41} \) | 377.15 [4] |
|59 | \( R = \text{C}_6\text{H}_{13} \) | 385.15 [4] |
|60 | \( R = \text{C}_{14}\text{H}_{29} \) | 368.15 [4] |
|61 | \( R = \text{C}_{20}\text{H}_{41} \) | 368.15 [4] |
|62 | ![Structure](image2) | 352.15 [4] |
|63 | \( X = \text{H}, Y = \text{H} \) | 448.35 [5] |
|64 | \( X = \text{H}, Y = \text{Cl} \) | 417.45 [5] |
|65 | \( X = \text{F}, Y = \text{H} \) | 423.65 [5] |
|66 | \( X = \text{F}, Y = \text{Cl} \) | 416.05 [5] |
|   | Structure Image | R = C\_xH\_y | Mass [Da] | Reference |
|---|-----------------|--------------|-----------|-----------|
| 67 | ![Structure 1](image1) | C\_6H\_17 | 388.15 | [6] |
| 68*| ![Structure 2](image2) | C\_10H\_21 | 378.15 | [6] |
| 69 | ![Structure 3](image3) | C\_12H\_25 | 375.15 | [6] |
| 70 | ![Structure 4](image4) | C\_14H\_29 | 374.15 | [6] |
| 71 | ![Structure 5](image5) | C\_16H\_33 | 378.15 | [6] |
| 72 | ![Structure 1](image1) | C\_6H\_17 | 386.15 | [6] |
| 73 | ![Structure 2](image2) | C\_10H\_21 | 368.15 | [6] |
| 74 | ![Structure 3](image3) | C\_12H\_25 | 366.15 | [6] |
| 75 | ![Structure 4](image4) | C\_14H\_29 | 368.15 | [6] |
| 76*| ![Structure 5](image5) | C\_16H\_33 | 371.15 | [6] |
| 77 | ![Structure 1](image1) | C\_16H\_33 | 395.15 | [6] |
| 78 | ![Structure 2](image2) | C\_6H\_13 | 399.15 | [7] |
| 79 | ![Structure 3](image3) | C\_8H\_17 | 392.15 | [7] |
| 80 | ![Structure 4](image4) | C\_10H\_21 | 379.15 | [7] |
| 81*| ![Structure 5](image5) | C\_12H\_25 | 379.15 | [7] |
| 82*| ![Structure 1](image1) | C\_14H\_29 | 381.15 | [7] |
| 83 | ![Structure 2](image2) | C\_16H\_33 | 373.15 | [7] |
| 84 | ![Structure 3](image3) | C\_18H\_53 | 384.15 | [7] |
|   | Chemical Structure | Molecular Weight | References |
|---|-------------------|------------------|------------|
| 85 | ![Chemical Structure 85](image) | 393.15 | [7] |
| 86 | ![Chemical Structure 86](image) | 387.15 | [7] |
| 87*| ![Chemical Structure 87*](image) | 363.15 | [7] |
| 88 | ![Chemical Structure 88](image) | R = C₈H₁₇, 416.15 | [8] |
| 89 | ![Chemical Structure 89](image) | R = C₁₀H₂₁, 409.15 | [8] |
| 90 | ![Chemical Structure 90](image) | R = C₁₂H₂₅, 410.15 | [8] |
| 91 | ![Chemical Structure 91](image) | R = C₁₄H₂₉, 412.15 | [8] |
| 92 | ![Chemical Structure 92](image) | R = C₁₆H₃₃, 413.15 | [8] |
| 93 | ![Chemical Structure 93](image) | R = C₁₈H₃₇, 415.15 | [8] |
| 94 | ![Chemical Structure 94](image) | R = C₈H₁₇, 389.15 | [9] |
| 95 | ![Chemical Structure 95](image) | R = C₁₀H₂₁, 389.15 | [9] |
| 96 | ![Chemical Structure 96](image) | R = C₁₂H₂₅, 387.15 | [9] |
| 97*| ![Chemical Structure 97*](image) | R = C₁₄H₂₉, 389.15 | [9] |
| 98 | ![Chemical Structure 98](image) | R = C₁₂H₂₅; R₁ = C₁₆H₃₃, 393.45 | [10] |
| 99 | ![Chemical Structure 99](image) | R = C₁₆H₃₃; R₁ = C₁₂H₂₅, 393.25 | [10] |
| 100| ![Chemical Structure 100](image) | R = C₁₆H₃₃; R₁ = C₁₆H₃₃, 391.75 | [10] |
|    | Structure | R   | Molecular Weight | Reference |
|----|-----------|-----|------------------|-----------|
| 101| ![Structure](image1) | R = C₃H₁₁ | 401.15 | [10] |
| 102|           | R = C₆H₁₃ | 420.35 | [10] |
| 103|           | R = C₇H₁₅ | 397.85 | [10] |
| 104|           | R = C₈H₁₇ | 388.05 | [10] |
| 105|           | R = C₉H₁₉ | 389.55 | [10] |
| 106|           | R = C₁₁H₂₃ | 393.25 | [10] |
| 107|           | R = C₁₂H₂₅ | 389.75 | [10] |
| 108|           | R = C₁₄H₂₉ | 388.75 | [10] |
| 109|           | R = C₁₆H₃₃ | 388.55 | [10] |
| 110| ![Structure](image2) | R = C₄H₉ | 437.75 | [11] |
| 111|           | R = C₅H₁₁ | 436.75 | [11] |
| 112|           | R = C₆H₁₃ | 437.25 | [11] |
| 113|           | R = C₇H₁₅ | 436.25 | [11] |
| 114|           | R = C₈H₁₇ | 437.15 | [11] |
| 115|           | R = C₉H₁₉ | 437.45 | [11] |
| 116|           | R = C₁₀H₂₁ | 436.85 | [11] |
| 117*|          | R = C₁₁H₂₃ | 436.25 | [11] |
| 118|           | R = C₁₂H₂₅ | 436.35 | [11] |
| 119|           | R = C₁₄H₂₉ | 435.25 | [11] |
| 120|           | R = C₁₆H₃₃ | 433.95 | [11] |
| 121| ![Structure](image3) | R = C₄H₉ | 420.45 | [11] |
| 122|           | R = C₅H₁₁ | 420.45 | [11] |
| 123|           | R = C₆H₁₃ | 422.45 | [11] |
| 124*|          | R = C₇H₁₅ | 421.05 | [11] |
| 125*|          | R = C₈H₁₇ | 419.85 | [11] |
| 126|           | R = C₉H₁₉ | 421.65 | [11] |
| 127|           | R = C₁₀H₂₁ | 422.65 | [11] |
| 128|           | R = C₁₁H₂₃ | 423.15 | [11] |
| 129|           | R = C₁₂H₂₅ | 423.65 | [11] |
| 130|           | R = C₁₄H₂₉ | 424.85 | [11] |
| 131|           | R = C₁₆H₃₃ | 422.15 | [11] |
|   | Chemical Structure | R               | Mass   | Reference |
|---|--------------------|-----------------|--------|-----------|
|132| ![Chemical Structure](image1) | R = OC₄H₉ | 394.65 | [12]      |
|133| ![Chemical Structure](image2) | R = OC₆H₁₃ | 395.15 | [12]      |
|134| ![Chemical Structure](image3) | R = OC₈H₁₇ | 393.55 | [12]      |
|135| ![Chemical Structure](image4) | R = OC₁₀H₂₁ | 393.95 | [12]      |
|136| ![Chemical Structure](image5) | R = OC₁₂H₂₅ | 396.05 | [12]      |
|137| ![Chemical Structure](image6) | R = C₄H₉   | 399.55 | [12]      |
|138| ![Chemical Structure](image7) | R = C₆H₁₃ | 394.65 | [12]      |
|139| ![Chemical Structure](image8) | R = C₈H₁₇ | 390.45 | [12]      |
|140| ![Chemical Structure](image9) | R = C₁₀H₂₁ | 388.95 | [12]      |
|141| ![Chemical Structure](image10) | R = C₁₂H₂₅ | 388.65 | [12]      |
|142| ![Chemical Structure](image11) | R = C₄H₉   | 418.95 | [13]      |
|143| ![Chemical Structure](image12) | R = C₆H₁₃ | 415.25 | [13]      |
|144| ![Chemical Structure](image13) | R = C₈H₁₇ | 413.65 | [13]      |
|145| ![Chemical Structure](image14) | R = C₁₀H₂₁ | 409.55 | [13]      |
|146| ![Chemical Structure](image15) | R = C₁₂H₂₅ | 409.05 | [13]      |
|147| ![Chemical Structure](image16) | R = OC₄H₉ | 431.55 | [13]      |
|148| ![Chemical Structure](image17) | R = OC₆H₁₃ | 430.35 | [13]      |
|149| ![Chemical Structure](image18) | R = OC₈H₁₇ | 426.55 | [13]      |
|150| ![Chemical Structure](image19) | R = OC₁₀H₂₁ | 420.15 | [13]      |
|151| ![Chemical Structure](image20) | R = OC₁₂H₂₅ | 415.95 | [13]      |
|152| ![Chemical Structure](image21) | R = C₈H₁₇ | 407.75 | [14]      |
|153| ![Chemical Structure](image22) | R = C₁₀H₂₁ | 405.45 | [14]      |
|154| ![Chemical Structure](image23) | R = C₁₂H₂₅ | 404.25 | [14]      |
|155| ![Chemical Structure](image24) | R = C₈H₁₇ | 414.15 | [15]      |
|156| ![Chemical Structure](image25) | R = C₁₀H₂₁ | 401.15 | [15]      |
|   | R = C_{12}H_{25}  | 398.15 [15] |
|---|------------------|-------------|
| 158 | R = C_{14}H_{29}  | 397.15 [15] |
| 159 | R = C_{16}H_{33}  | 394.15 [15] |

![Diagram 1]

|   | R = OC_{5}H_{11}  | 454.15 [16] |
|---|------------------|-------------|
| 160 | R = OC_{6}H_{13}  | 446.55 [16] |
| 161 | R = OC_{7}H_{15}  | 444.85 [16] |
| 162 | R = OC_{8}H_{17}  | 447.05 [16] |
| 163 | R = OC_{10}H_{21} | 446.05 [16] |
| 164 | R = OC_{12}H_{25} | 443.05 [16] |
| 165 | R = OC_{16}H_{33} | 436.85 [16] |
| 166 | R = C_{5}H_{11}   | 423.05 [16] |
| 167 | R = C_{6}H_{13}   | 428.75 [16] |
| 168 | R = C_{8}H_{17}   | 431.25 [16] |
| 169 | R = C_{10}H_{21}  | 431.65 [16] |
| 170 | R = C_{12}H_{25}  | 429.15 [16] |
| 171 | R = C_{14}H_{29}  | 424.45 [16] |

![Diagram 2]

|   | R = OC_{5}H_{15}  | 403.15 [16] |
|---|------------------|-------------|
| 173 | R = OC_{8}H_{17}  | 406.15 [16] |
| 174 | R = OC_{9}H_{19}  | 409.15 [16] |
| 175 | R = OC_{10}H_{21} | 413.15 [16] |
| 176 | R = OC_{12}H_{25} | 415.15 [16] |
| 177 | R = C_{5}H_{11}   | 392.15 [16] |
| 178 | R = C_{6}H_{13}   | 398.15 [16] |
| 179 | R = C_{8}H_{17}   | 400.15 [16] |
| 180 | R = C_{10}H_{21}  | 400.15 [16] |
| 181 | R = C_{12}H_{25}  | 400.15 [16] |

![Diagram 3]

|   | R = OC_{6}H_{13}  | 438.15 [16] |
|---|------------------|-------------|
| 182 | R = OC_{7}H_{15}  | 426.15 [16] |
| 183 | R = OC_{8}H_{17}  | 421.15 [16] |
| 184 | R = OC_{9}H_{19}  | 416.15 [16] |
| 185 | R = OC_{10}H_{21} | 415.15 [16] |
| No. | R         | H          | Molar Mass | Ref. |
|-----|-----------|------------|------------|------|
| 186 | R = OC\textsubscript{10}H\textsubscript{21} | 413.15     |            | [16] |
| 187 | R = OC\textsubscript{12}H\textsubscript{25} | 410.15     |            | [16] |
| 188 | R = C\textsubscript{14}H\textsubscript{29} | 390.15     |            | [16] |
| 189 | R = OC\textsubscript{7}H\textsubscript{15} | 446.15     |            | [16] |
| 190 | R = OC\textsubscript{8}H\textsubscript{17} | 445.15     |            | [16] |
| 191*| R = OC\textsubscript{9}H\textsubscript{19} | 441.15     |            | [16] |
| 192*| R = OC\textsubscript{10}H\textsubscript{21} | 440.15     |            | [16] |
| 193 | R = OC\textsubscript{12}H\textsubscript{25} | 437.15     |            | [16] |
| 194 | R = OC\textsubscript{6}H\textsubscript{13} | 450.15     |            | [16] |
| 195*| R = OC\textsubscript{7}H\textsubscript{15} | 449.15     |            | [16] |
| 196 | R = OC\textsubscript{8}H\textsubscript{17} | 450.15     |            | [16] |
| 197 | R = OC\textsubscript{9}H\textsubscript{19} | 447.15     |            | [16] |
| 198 | R = OC\textsubscript{12}H\textsubscript{25} | 446.15     |            | [16] |
| 199 | R = OC\textsubscript{6}H\textsubscript{13} | 421.15     |            | [16] |
| 200 | R = OC\textsubscript{7}H\textsubscript{15} | 409.15     |            | [16] |
| 201 | R = OC\textsubscript{8}H\textsubscript{17} | 405.15     |            | [16] |
| 202 | R = OC\textsubscript{9}H\textsubscript{19} | 395.15     |            | [16] |
| 203 | R = OC\textsubscript{10}H\textsubscript{21} | 390.15     |            | [16] |
| 204 | R = OC\textsubscript{6}H\textsubscript{13} | 403.15     |            | [16] |
| 205*| R = OC\textsubscript{7}H\textsubscript{15} | 399.15     |            | [16] |
| 206*| R = OC\textsubscript{8}H\textsubscript{17} | 397.15     |            | [16] |
| 207 | R = OC\textsubscript{9}H\textsubscript{19} | 390.15     |            | [16] |
| 208 | ![Structure](image) | 394.15 | [16] |
| 209 | ![Structure](image) | 420.15 | [16] |
| 210 | ![Structure](image) | 424.15 | [16] |
| 211 | ![Structure](image) | 458.15 | [16] |
| 212 | ![Structure](image) |
| 213 | R = OC$_{12}$H$_{25}$; R$_1$ = OC$_8$H$_{17}$ | 401.55 | [16] |
| 214 | R = OC$_{12}$H$_{25}$; R$_1$ = OC$_{10}$H$_{21}$ | 411.65 | [16] |
| 215 | R = OC$_{12}$H$_{25}$; R$_1$ = OC$_{11}$H$_{23}$ | 412.15 | [16] |
| 216 | R = OC$_{12}$H$_{25}$; R$_1$ = OC$_{12}$H$_{25}$ | 414.15 | [16] |
| 217 | R = OC$_{12}$H$_{25}$; R$_1$ = OC$_{13}$H$_{27}$ | 414.65 | [16] |
| 218 | R = OC$_{12}$H$_{25}$; R$_1$ = OC$_{14}$H$_{29}$ | 415.15 | [16] |
| 219 | R = OC$_{10}$H$_{21}$; R$_1$ = OC$_8$H$_{17}$ | 407.15 | [16] |
| 220 | R = OC$_{10}$H$_{21}$; R$_1$ = OC$_9$H$_{19}$ | 407.15 | [16] |
| 221 | R = OC$_{10}$H$_{21}$; R$_1$ = OC$_{10}$H$_{21}$ | 405.15 | [16] |
| 222 | ![Structure](image) |
| 223* | R = C$_{12}$H$_{25}$ | 387.55 | [17] |
| 223* | R = C$_{13}$H$_{27}$ | 379.95 | [17] |
| 224* | R = OC₈H₁₇ | 426.05 | [17] |
| 225 | R = C₁₀H₂₁ | 412.75 | [17] |
| 226 | R = C₁₁H₂₃ | 409.55 | [17] |
| 227 | R = C₁₂H₂₅ | 410.45 | [17] |
| 228 | R = C₁₃H₂₇ | 421.95 | [17] |

| 229 | R = OC₈H₁₇ | 432.85 | [17] |
| 230 | R = C₁₀H₂₁ | 425.65 | [17] |
| 231 | R = C₁₁H₂₃ | 427.15 | [17] |
| 232 | R = C₁₂H₂₅ | 424.85 | [17] |
| 233* | R = C₁₃H₂₇ | 424.15 | [17] |

| 234 | R = C₇H₁₅ | 414.65 | [18] |
| 235 | R = C₈H₁₇ | 415.65 | [18] |
| 236 | R = C₉H₁₉ | 416.15 | [18] |
| 237* | R = C₁₀H₂₁ | 415.65 | [18] |
| 238* | R = C₁₁H₂₃ | 415.65 | [18] |
| 239 | R = C₁₂H₂₅ | 413.65 | [18] |
| 240 | R = C₁₃H₂₇ | 413.65 | [18] |
| 241 | R = C₁₄H₂₉ | 412.15 | [18] |
| 242 | R = C₁₆H₃₃ | 411.65 | [18] |
| 243* | R = C₁₈H₃₇ | 409.15 | [18] |

* Compounds used in test set
References

1. Srinivasan MV, Kannan P, Roy A. Photo and electrically switchable B7 mesophase exhibiting asymmetric bent-core liquid crystals. New J Chem. 2013;37:1584–1590.

2. Nagaveni NG, Roy A, Prasad V. Achiral bent-core azo compounds: effect of different types of linkage groups and their direction of linking on liquid crystalline properties. J Mater Chem. 2012;22:8948–8959.

3. Vijay Srinivasan M, Kannan P, Roy A. Investigations on photo and electrically switchable asymmetric bent-core liquid crystals. J Mater Sci. 2013;48:2433–2446.

4. Alaasar M, Prehm M, Brautzsch M, Tschiertske C. 4-Methylresorcinol based bent-core liquid crystals with azobenzene wings – a new class of compounds with dark conglomerate phases. J Mater Chem C. 2014;2:5487–5501.

5. Lutfor MR, Hegde G, Kumar S, Tschiertske C, Chigrinov VG. Synthesis and characterization of bent-shaped azobenzene monomers: Guest-host effects in liquid crystals with azo dyes for optical image storage devices. Opt Mater. 2009;32:176–183.

6. Alaasar M, Prehm M, Tschiertske C. Influence of halogen substituent on the mesomorphic properties of five-ring banana-shaped molecules with azobenzene wings. Liq Cryst. 2013;40:656–668.

7. Alaasar M, Prehm M, Brautzsch M, Tschiertske C. Dark conglomerate phases of azobenzene derived bent-core mesogens – relationships between the molecular structure and mirror symmetry breaking in soft matter. Soft Matter. 2014;10:7285–7296.

8. Alaasar M, Prehm M, May K, Eremin A, Tschiertske C. 4-Cyanoresorcinol-based bent-core mesogens with azobenzene wings: Emergence of sterically stabilized polar order in liquid crystalline phases. Adv Funct Mater. 2014;24:1703–1717.

9. Alaasar M, Prehm M, Tschiertske C. A new room temperature dark conglomerate mesophase formed by bent-core molecules combining 4-iodoresorcinol with azobenzene units. Chem Commun. 2013;49:11062–11064.

10. Nagaveni NG, Raghuvanshi P, Roy A, Prasad V. Azo-functionalised achiral bent-core liquid crystalline materials: effect of presence of –N=N– linkage at different locations in the molecular architecture. Liq Cryst. 2013;40:1238–1254.

11. Nagaveni NG, Prasad V, Roy A. Azo functionalised achiral bent-core liquid crystals: observation of photo-induced effects in B7 and B2 mesophases. Liq Cryst. 2013;40:1405–1416.

12. Prasad V, Kang S-W, Qi X, Kumar S. Photo-responsive and electrically switchable mesophases in a novel class of achiral bent-core azo compounds. J Mater Chem. 2004;14:1495–1502.

13. Prasad V, Kang S-W, Kumar S. Novel examples of achiral bent-core azo compounds exhibiting B1 and anticlinic-antiferroelectric B2 mesophases. J Mater Chem.
14. Prasad V, Jákli A. Achiral bent-core azo compounds: observation of photoinduced effects in an antiferroelectric tilted smectic mesophase. Liq Cryst. 2004;31:473–479.

15. Alaasar M, Prehm M, Tschierske C. New azobenzene containing bent-core liquid crystals based on disubstituted resorcinol. Liq Cryst. 2014;41:126–136.

16. Pelzl G, Diele S, Weissflog W. Banana-shaped compounds - a new field of liquid crystals. Adv Mater. 1999;11:707–724.

17. Pyc P, Mieczkowski J, Pociecha D, Gorecka E, Donnio B, Guillon D. Bent-core molecules with lateral halogen atoms forming tilted, synclinic and anticlinic, lamellar phases. J Mater Chem. 2004;14:2374–2379.

18. Umadevi S, Jákli A, Sadashiva BK. Odd-even effects in bent-core compounds containing terminal n-alkyl carboxylate groups. Soft Matter. 2006;2:875–885.