Supporting Information

Naturally Occurring Polyphenols as Building Blocks for Supramolecular Liquid Crystals – Substitution Pattern Dominates Mesomorphism

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Materials and Methods

The chalconoids and stilbenoids were purchased from TCI or Sigma Aldrich and used without further purification. POM (Polarized optical microscopy) were taken on a *Nikon Eclipse* Ni equipped with combined with a *Linkam* heating station and an OPTIX-CAM SUMNIT 2K camera. A heating rate of 10 K/min was used. Given temperature values in the POM images show the actual temperature at which the images were taken. DSC traces were recorded with a *Mettler Toledo* DSC3+. Samples (2-5 mg) were heated with a rate of 10 K/min and argon was used as flushing gas with a flow of 20 mL/min.

Samples were measured three times. IR-spectra were measured on a *Bruker* Alpha Platinum equipped with an ATR crystal.

Synthesis of Hydrogen-Bond Acceptors

St₈ was synthesized following a known literature protocol. All spectra were in accordance with those reported before.^[1]

 Ap_8 was synthesized following a known literature protocol. All spectra were in accordance with those reported before.^[2]

Synthesis of the hydrogen-bonded complexes

All HBAs were obtained by weighing the hydrogen bond donator and 3 equivalents of the hydrogen bond acceptor in separate vials. After dissolving both in acetone, the solutions were mixed and the solvent was slowly evaporated to form the hydrogenbonded assemblies.

Melting points of the starting material

| compound name | mp. | | | | |
|-------------------|----------------------------------|--|--|--|--|
| Res | 253 °C (decomposition) | | | | |
| Оху | 201 – 205,5 °C | | | | |
| Pic | 235 °C (decomposition) 215 °C | | | | |
| But | | | | | |
| lso | 207 – 210 °C | | | | |
| St-C ₈ | 92 °C | | | | |
| Ap-C ₈ | 69 °C | | | | |

ESI Tab. 1: melting points of the starting materials.

IR-spectra







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Fig S1: IR spectra of the HB-assemblies of all possible stoichiometric ratios (black), the hydrogen bond acceptor (red) and the hydrogen bond donator (blue). The IR spectra of **Res(Ap**₈)₃ and **Res(St**₈)₃ were reported before and are shown for comparison reasons

Polarized optical microscopy



Fig S2: POM pictures taken on cooling the HB-assembly **Res(St**₈)₁ under crossed polarizers. A) isotropic state, B) nematic-phase, C) glassy state preserving the liquid crystalline state.



Fig S3: POM pictures taken on cooling the HB-assembly **Res(St**₈)₂ under crossed polarizers. A) isotropic state, B) nematic-phase, C) glassy state preserving the liquid crystalline state.



Fig S4: POM pictures taken on cooling the HB-assembly **Res(Ap₈)**² under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S5: POM pictures taken on cooling the HB-assembly $\text{Res}(\text{St}_8)_3$ under crossed polarizers. A) isotropic state, B) nematic-phase, C) glassy state preserving the liquid crystalline state. This system has been reported before and is shown for comparative reasons.^[3]



Fig S6: POM pictures taken on cooling the HB-assembly **Res(Ap₈)**₃ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline phase. This system has been reported before and is shown for comparative reasons.^[3]



Fig S7: POM pictures taken on cooling the HB-assembly **Oxy(St**₈)₄ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.







Fig S8: POM pictures taken on cooling the HB-assembly **Oxy(Ap**₈)₄ under crossed polarizers. A) isotropic state, B) nematic-phase forming while the sample crystallizes, C) crystalline state.







Fig S9: POM pictures taken on cooling the HB-assembly **Oxy(St₈)**³ under crossed polarizers. A) isotropic state, B) nematic-phase, C) smectic-phase.



Fig S10: POM pictures taken on cooling the HB-assembly **Oxy(Ap₈)**³ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline phase.



Fig S11: POM pictures taken on cooling the HB-assembly **Oxy(St₈)**₂ under crossed polarizers. A) isotropic state, B) nematic-phase, C) smectic-phase.







Fig S12: POM pictures taken on cooling the HB-assembly **Oxy(Ap**₈)₂ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline phase.







Fig S13: POM pictures taken on cooling the HB-assembly **Pic(St**₈)₄ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S14: POM pictures taken on cooling the HB-assembly **Pic(Ap₈)**₄ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S15: POM pictures taken on cooling the HB-assembly **Pic(St**₈)₃ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.







Fig S16: POM pictures taken on cooling the HB-assembly **Pic(Ap₈)**₃ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.

A) 156 °C







Fig S17: POM pictures taken on cooling the HB-assembly **Pic(St₈)**₂ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S18: POM pictures taken on cooling the HB-assembly **Pic(Ap₈)**₂ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S19: POM pictures taken on cooling the HB-assembly **Pic(St**₈)₁ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.







Fig S20: POM pictures taken on cooling the HB-assembly **Pic(Ap₈)**₁ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.







Fig S21: POM pictures taken on cooling the HB-assembly **But(St**₈)₄ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S22: POM pictures taken on cooling the HB-assembly **But(Ap₈)**₄ under crossed polarizers. A) isotropic state, B) nematic-phase forming while the sample crystallizes, C) crystalline state.



Fig S23: POM pictures taken on cooling the HB-assembly **But(St₈)**₃ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.







Fig S24: POM pictures taken on cooling the HB-assembly **But(Ap₈)**₃ under crossed polarizers. A) isotropic state, B) nematic-phase while the sample starts to crystallize, C) crystalline state.



Fig S25: POM pictures taken on cooling the HB-assembly **But(St₈)**₂ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S26: POM pictures taken on cooling the HB-assembly **But(Ap₈)**₂ under crossed polarizers. A) isotropic state, B) crystalline state.



Fig S27: POM pictures taken on cooling the HB-assembly **But(St₈)**¹ under crossed polarizers. A) isotropic state, B) nematic-phase, C) glassy state preserving the liquid crystalline state.







Fig S28: POM pictures taken on cooling the HB-assembly **Iso(St₈)**³ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.







Fig S29: POM pictures taken on cooling the HB-assembly **Iso(Ap₈)**₃ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S30: POM pictures taken on cooling the HB-assembly **Iso(St₈)**² under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.



Fig S31: POM pictures taken on cooling the HB-assembly **Iso(Ap₈)**₂ under crossed polarizers. A) isotropic state, B) nematic-phase, C) crystalline state.







Fig S32: POM pictures taken on cooling the HB-assembly **Iso(St₈)**¹ under crossed olarizers. A) isotropic state, B) nematic-phase, C) glassy state preserving the liquid crystalline state.







Fig S33: POM pictures taken on cooling the HB-assembly **Iso(Ap₈)**¹ under crossed olarizers. A) isotropic state, B) nematic-phase, C) glassy state preserving the liquid crystalline state.

Differential scanning calometry

DSC plots of Res(St-C₈)₃ and Res(Ap-C₈)₃ have been reported before.^[3]



Fig S30: DSC curve of the HB-assembly Res(Ap₈)₁ measured with a heating/cooling rate of 10 °C/min.



25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 °C

Fig S31: DSC curve of the HB-assembly **Res(Ap**₈)₂ measured with a heating/cooling rate of 10 °C/min.



Fig S32: DSC curve of the HB-assembly $\text{Res}(\text{St}_8)_1$ measured with a heating/cooling rate of 10 °C/min.



Fig S33: DSC curve of the HB-assembly $Res(St_8)_2$ measured with a heating/cooling rate of 10 °C/min.



Fig S34: DSC curve of the HB-assembly **Iso(St**₈)₃ measured with a heating/cooling rate of 10 °C/min.



Fig S35: DSC curve of the HB-assembly $Iso(St_8)_2$ measured with a heating/cooling rate of 10 °C/min.



Fig S36: DSC curve of the HB-assembly **Iso(St**₈) measured with a heating/cooling rate of 10 °C/min.



Fig S37: DSC curve of the HB-assembly Iso(Ap₈)₃ measured with a heating/cooling rate of 10 °C/min.



Fig S38: DSC curve of the HB-assembly **Iso(Ap**₈)₂ measured with a heating/cooling rate of 10 °C/min.

Fig S39: DSC curve of the HB-assembly **Iso(Ap**₈) measured with a heating/cooling rate of 10 °C/min.

30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190

Fig S40: DSC curve of the HB-assembly $Oxy(St_8)_4$ measured with a heating/cooling rate of 10 °C/min.

200 °C

Fig S41: DSC curve of the HB-assembly $Oxy(St_8)_3$ measured with a heating/cooling rate of 10 °C/min.

Fig S42: DSC curve of the HB-assembly $Oxy(St_8)_2$ measured with a heating/cooling rate of 10 °C/min.

Fig S43: DSC curve of the HB-assembly **Oxy(St**₈) measured with a heating/cooling rate of 10 °C/min.

Fig S44: DSC curve of the HB-assembly Oxy(Ap₈)₄ measured with a heating/cooling rate of 10 °C/min.

Fig S45: DSC curve of the HB-assembly Oxy(Ap₈)₃ measured with a heating/cooling rate of 10 °C/min.

25 30 35 40 45 50 55 60 65 70 75 80 85 90 55 100 105 110 115 120 125 130 135 140 145 150 165 160 165 170 175 °C

Fig S46: DSC curve of the HB-assembly Oxy(Ap₈)₂ measured with a heating/cooling rate of 10 °C/min.

25

Fig S47: DSC curve of the HB-assembly **Oxy(Ap**₈) measured with a heating/cooling rate of 10 °C/min.

125 130

135 140 145 150 155 160 165 170

Fig S48: DSC curve of the HB-assembly **But(St**₈)₄ measured with a heating/cooling rate of 10 °C/min.

25 30 25 40 45 50 55 60 65 70 75 80 85 90 95 100 165 110 115 120 125 130 135 °C

Fig S49: DSC curve of the HB-assembly $But(St_8)_3$ measured with a heating/cooling rate of 10 °C/min.

Fig S50: DSC curve of the HB-assembly **But(St**₈)₂ measured with a heating/cooling rate of 10 °C/min.

Fig S51: DSC curve of the HB-assembly **But(St**₈) measured with a heating/cooling rate of 10 °C/min.

Fig S52: DSC curve of the HB-assembly **But(Ap**₈)₄ measured with a heating/cooling rate of 10 °C/min.

Fig S53: DSC curve of the HB-assembly **But(Ap**₈)₃ measured with a heating/cooling rate of 10 °C/min.

Fig S54: DSC curve of the HB-assembly **But(Ap**₈)₂ measured with a heating/cooling rate of 10 °C/min.

Fig S55: DSC curve of the HB-assembly **But(Ap**₈) measured with a heating/cooling rate of 10 °C/min.

Fig S56: DSC curve of the HB-assembly **Pic(St**₈)₄ measured with a heating/cooling rate of 10 °C/min.

Fig S57: DSC curve of the HB-assembly **Pic(St**₈)₃ measured with a heating/cooling rate of 10 °C/min.

Fig S58: DSC curve of the HB-assembly **Pic(St**₈)₂ measured with a heating/cooling rate of 10 °C/min.

Fig S59: DSC curve of the HB-assembly $Pic(St_8)$ measured with a heating/cooling rate of 10 °C/min.

Fig S60: DSC curve of the HB-assembly **Pic(Ap**₈)₄ measured with a heating/cooling rate of 10 °C/min.

Fig S61: DSC curve of the HB-assembly **Pic(Ap**₈)₃ measured with a heating/cooling rate of 10 °C/min.

Fig S62: DSC curve of the HB-assembly **Pic(Ap**₈)₂ measured with a heating/cooling rate of 10 °C/min.

Fig S63: DSC curve of the HB-assembly **Pic(Ap**₈) measured with a heating/cooling rate of 10 °C/min.

Single-crystal X-ray analyses.

Pic(St₈)₃

 $[C_{77}\,H_{93}\,N_3\,O_7]$: A colorless plate-like specimen of $\text{Pic}(\text{St}_8)_3$, approximate dimensions 0.030 mm x 0.100 mm x 0.330 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a triclinic unit cell yielded a total of 14859 reflections to a maximum q angle of 25.00° (0.84 Å resolution), of which 11419 were independent (average redundancy 1.301, completeness = 97.9%, R_{int} = 5.30%, R_{sig} = 6.01%) and 8112 (71.04%) were greater than $2s(F^2)$. The final cell constants of <u>a</u> = 11.0932(3) Å, <u>b</u> = 11.2131(4) Å, <u>c</u> = 27.2387(8) Å, a = 96.3970(10)°, b = 98.6070(10)°, g = 95.688(3)°, volume = 3305.99(18) Å³, are based upon the refinement of the XYZ-centroids of reflections above 20 s(I). Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9760 and 0.9980.

The structure was solved and refined using the Bruker SHELXTL Software Package^[4], using the space group P -1, with Z = 2 for the formula unit, C77H93N3O7. The final anisotropic full-

matrix least-squares refinement on F² with 950 variables converged at R1 = 7.21%, for the observed data and wR2 = 16.99% for all data. The goodness-of-fit was 1.112. The largest peak in the final difference electron density synthesis was 0.181 e⁻/Å³ and the largest hole was - 0.192 e⁻/Å³ with an RMS deviation of 0.041 e⁻/Å³. On the basis of the final model, the calculated density was 1.178 g/cm³ and F(000), 1264 e⁻.

CCDC Number: 1942435

Pic(Ap₈)₃

Single-crystal X-ray analyses. The crystals were mounted on nylon loops in inert oil. Data of $Pic(Ap_8)_3$ were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated MoK α radiation, $\lambda = 0.71073$ Å) at 100(2) K .The structures were solved by Direct Methods (SHELXS-97)^[4a] and refined anisotropically by full-matrix least-squares on F² (SHELXL-2014)^[4b, 4c]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX2/3). Hydrogen atoms were refined using a riding model or rigid methyl groups. OH hydrogen atoms were refined freely. One half of the picetannol residue is disordered over two positions. RIGU and ISOR restraints were applied to the ADP of the corresponding atoms.

CCDC Number: 1945777

Calculations

For the calculations a computer with an Intel® Core[™] i7-8750H Processor and 16 GB RAM and the *CrystalExplorer* program was used.^[5] The energies were calculated using the option "accurate". Here a cluster of molecules within a radius of 3.8 Å from the reference molecule was considered.

See http://130.95.176.70/wiki/index.php/Intermolecular_Interaction_Energies for further details.

As explained in the main text of the manuscript, our structures are disordered. Since the data collection was performed at very low temperature (100 K) it is a reasonable approximation to take the structure of the most populated conformer as the starting point for the calculation, and to consider the disorder as static. We have shown in a previous investigation that our approximation yields accurate results.^[6]

Details on Structure Determinants

Below we give a chart, which explain the information given in the ESI Table 2 and 3.

| | Ν | Symop | R | Electron Density | E_ele | E_pol | E_dis | E_rep | E_tot |
|---|---|-------|---|------------------|-------|-------|-------|-------|-------|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |

1) Structure Determinant color, as provided in Fig. 5 and 6 in the manuscript

2) The number of pairs, N, in the graphics window with that energy.

3) Symmetry operator joining the two molecules in the pair.

4) Distance between centers of mass of both molecules (Å).

5) Level of theory at which the electron density is computed: B3LYP/6-31G(d,p) here.

6) Electrostatic contribution (kJ/mol).

7) Polarization contribution (kJ/mol).

8) Dispersion contribution (kJ/mol).

9) Repulsion contribution (kJ/mol).

10) Total energy (kJ/mol): This is the *sum of scaled components* (using the scale factors appropriate to the model as given below), but the *separate components are not scaled*.

| Energy Model | k_ele | k_pol | k_disp | k_rep |
|---|-------|-------|--------|-------|
| CE-B3LYP, B3LYP/6-31G(d,p) electron densities | 1.057 | 0.740 | 0.871 | 0.618 |

| Ν | Symop | R | Electron Density | E_ele | E_pol | E_dis | E_rep | E_tot |
|---|-------|-------|------------------|-------|-------|-------|-------|-------|
| 2 | - | 7.28 | B3LYP/6-31G(d,p) | -34.8 | -8.3 | -17.4 | 43.8 | -31.1 |
| 1 | - | 6.95 | B3LYP/6-31G(d,p) | -8.3 | -3.0 | -50.2 | 32.4 | -34.6 |
| 1 | - | 16.69 | B3LYP/6-31G(d,p) | -59.1 | -13.6 | -13.1 | 76.6 | -36.6 |
| 1 | - | 15.96 | B3LYP/6-31G(d,p) | -66.4 | -16.2 | -14.8 | 82.3 | -44.2 |
| 1 | - | 16.89 | B3LYP/6-31G(d,p) | -66.1 | -16.4 | -12.4 | 77.5 | -44.9 |
| 1 | - | 7.17 | B3LYP/6-31G(d,p) | -12.5 | -2.6 | -53.1 | 28.9 | -43.5 |

ESI Tab. 2: Pic(Ap₈)₃ energy decomposition

ESI Tab. 3: Pic(St₈)₃energy decomposition

| Ν | Symop | R | Electron Density | E_ele | E_pol | E_dis | E_rep | E_tot |
|---|-------|-------|------------------|-------|-------|-------|-------|-------|
| 1 | - | 7.70 | B3LYP/6-31G(d,p) | -6.4 | -2.3 | -50.8 | 34.3 | -31.7 |
| 1 | - | 16.31 | B3LYP/6-31G(d,p) | -75.5 | -19.3 | -12.5 | 92.4 | -44.8 |
| 1 | - | 6.18 | B3LYP/6-31G(d,p) | -13.5 | -2.7 | -63.2 | 42.3 | -30.3 |
| 1 | - | 7.41 | B3LYP/6-31G(d,p) | -7.2 | -2.9 | -50.2 | 32.4 | -34.7 |
| 1 | - | 15.02 | B3LYP/6-31G(d,p) | -73.7 | -18.8 | -14.6 | 83.8 | -46.2 |
| 1 | - | 10.42 | B3LYP/6-31G(d,p) | -60.4 | -14.3 | -13.2 | 77.0 | -39.0 |

SAXS and WAXS measurements

The structure of the liquid crystalline mesophases were studied by small (SAXS) and wide angle X-ray scattering (WAXS). Measurements were done at a self-constructed instrument using a rotating anode x-ray generator (Rigaku MicroMax 007), multilayer optics (Osmic Confocal Max-Flux, Cu K α , λ =1.54 Å).^[7] Samples were contained in 1 mm thick glass capillaries and measured in transmission geometry. Temperatures were controlled by a hot compressed air stream (Leister, LE MINI SENSOR). A permanent magnet (AlNiCo, 2000 Gauss) was used for alignment of the nematic phase. 2D scattering data was recorded on an online image plate detector (Mar345) at 352 mm sample to detector distance. Diffraction patterns, *l*(*q*) vs. total scattering vector *q* = 4 $\pi/\lambda \sin(\theta)$, where 2 θ is the scattering angle, (Fig. 4, manuscript) were obtained by radial averaging of the 2D scattering data using the analysis software Datasqueeze developed by P.A. Heiney.^[8]

Fig. S64: Radial average of the SAXS/WAXS patterns of **Oxy(St**₈)₃ in a smectic (A), nematic (B) and isotropic (C) phase.

Fig. S65: Integrated SAXS intensities of the scattering peak associated to the long ($q_1 = 0.146 \text{ Å}^{-1}$) and short ($q_{11} = 1.4 \text{ Å}^{-1}$) distance in the nematic mesophase vs. azimuthal angle chi. The sample (**Oxy(St**_B)_3) was oriented in a magnetic field B pointing in the $\chi = 0^{\circ}$ (horizontal) direction.

Fig. S66: Molecular packing of **Pic** in the crystal lattice. The structure reveals intermolecular hydrogen bonding but no intramolecular. CCDC 706345^[9]

Fig. S66: Molecular packing of But in the crystal lattice. The structure reveals inter- and intramolecular hydrogen bonding. CCDC $1117309^{[10]}$

Fig. S67: Molecular packing of lso in the crystal lattice. The structure reveals inter- and intramolecular hydrogen bonding. CCDC 916410^[11]

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