Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information for

Useful Synthetic Artifacts? The Impact of Ubiquitous Linker-Adjacent Groups on the Self-Assembly of Discotic Dimers

Carson O. Zellmann-Parrotta[1] *and Vance E. Williams*[1]

[1]Department of Chemistry, Simon Fraser University, Burnaby, BC V5A 1S6, Canada

vancew@sfu.ca

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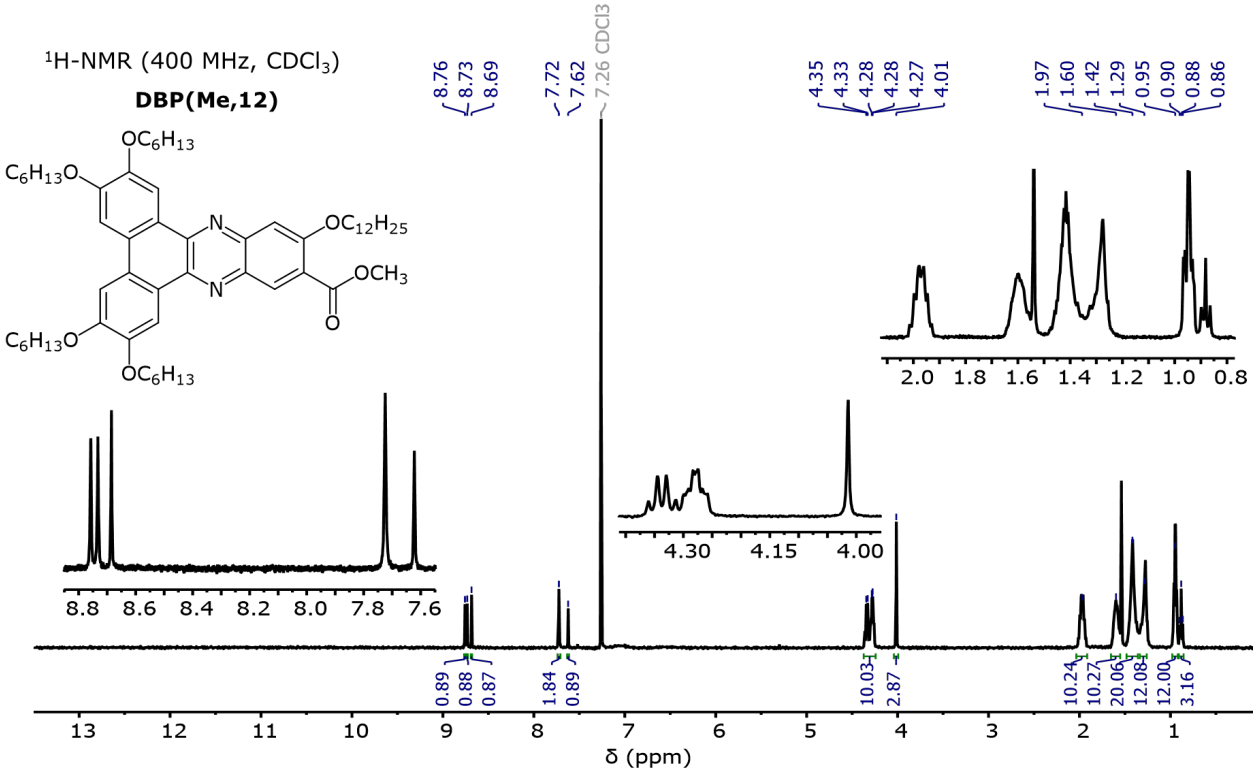
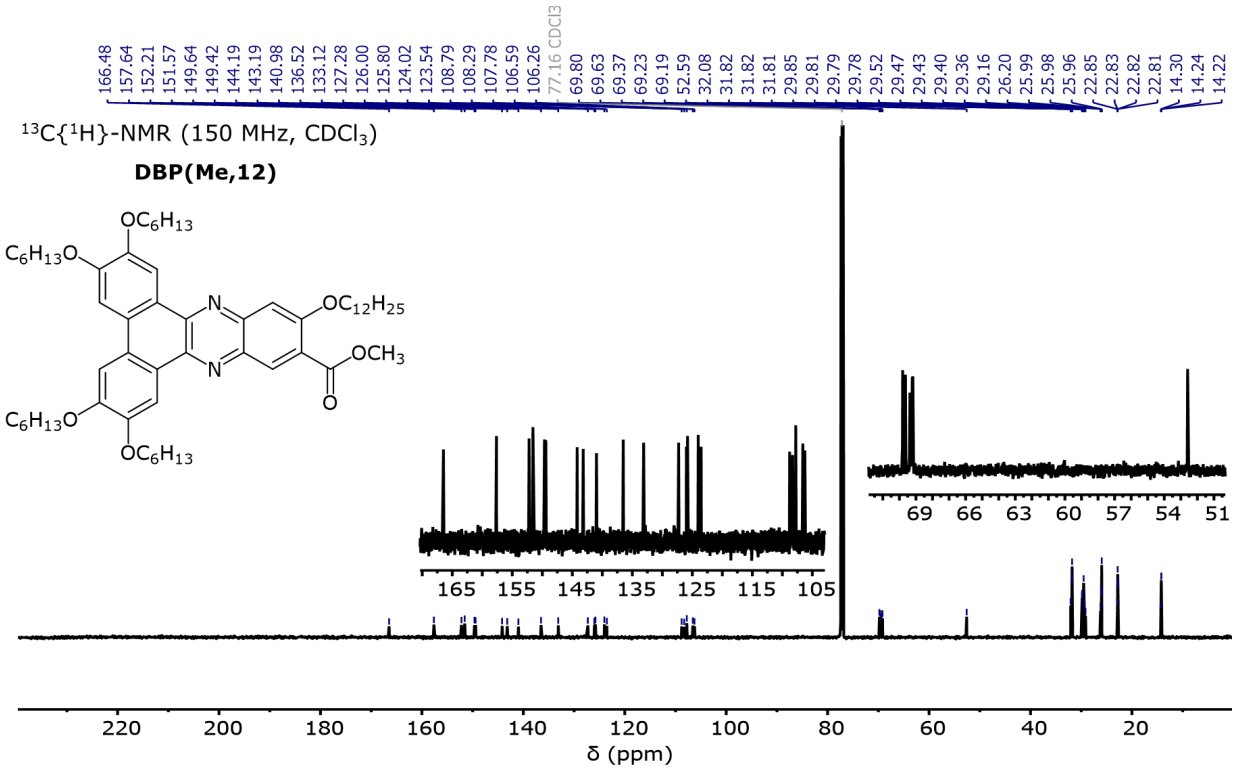


Figure S1. ^{1}H-NMR spectrum of **DBP(Me,12)**.



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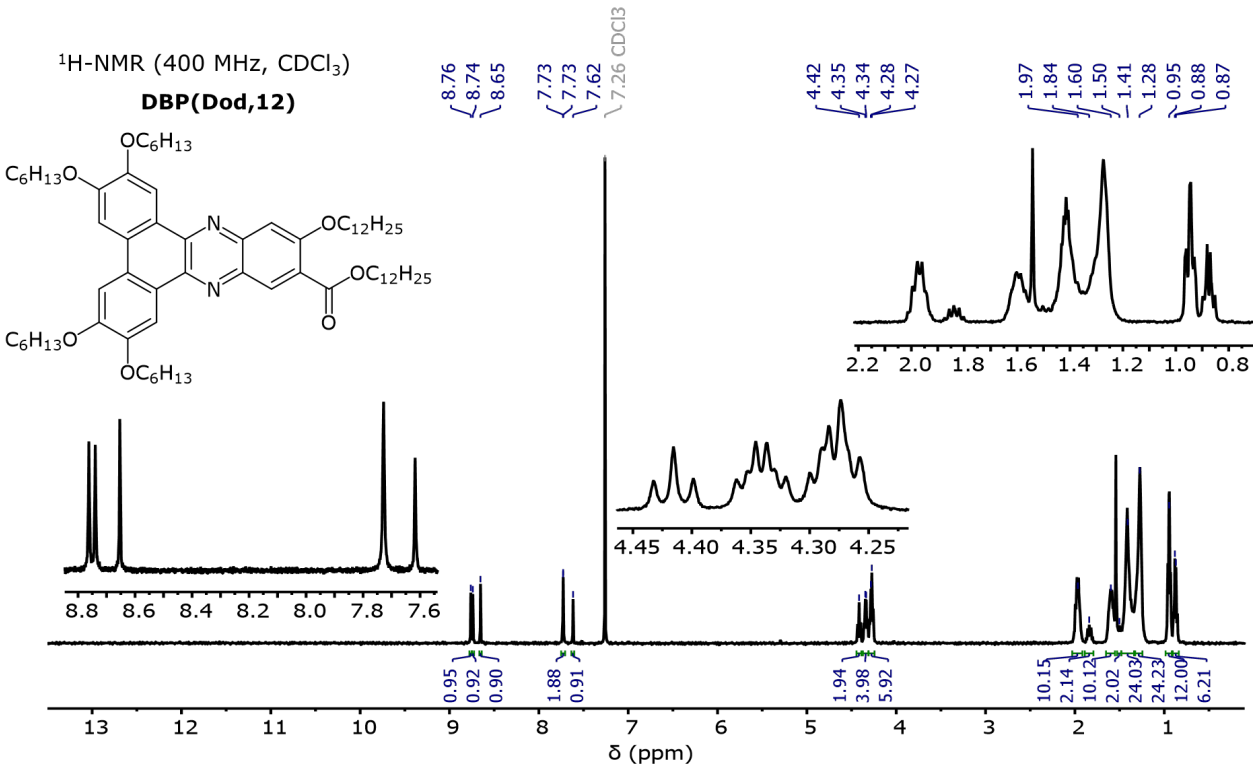


Figure S3. ^{1}H-NMR spectrum of **DBP(Dod,12)**.

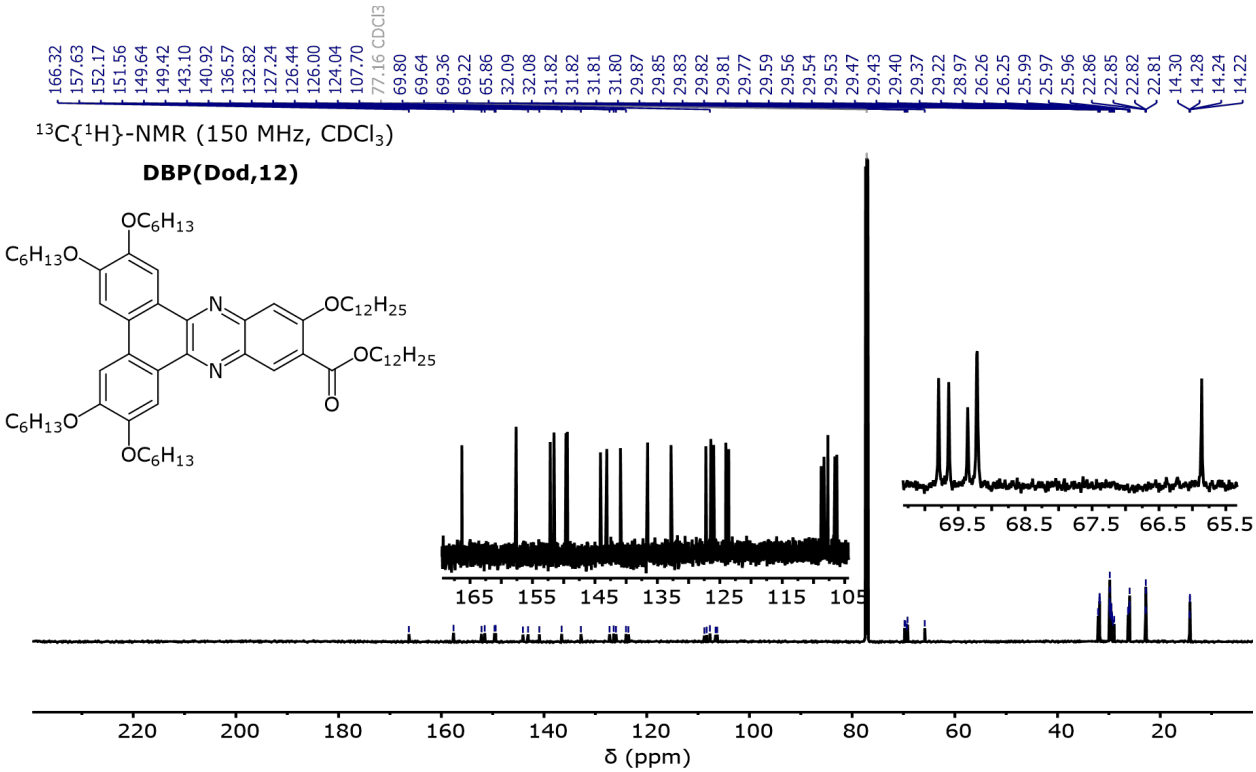
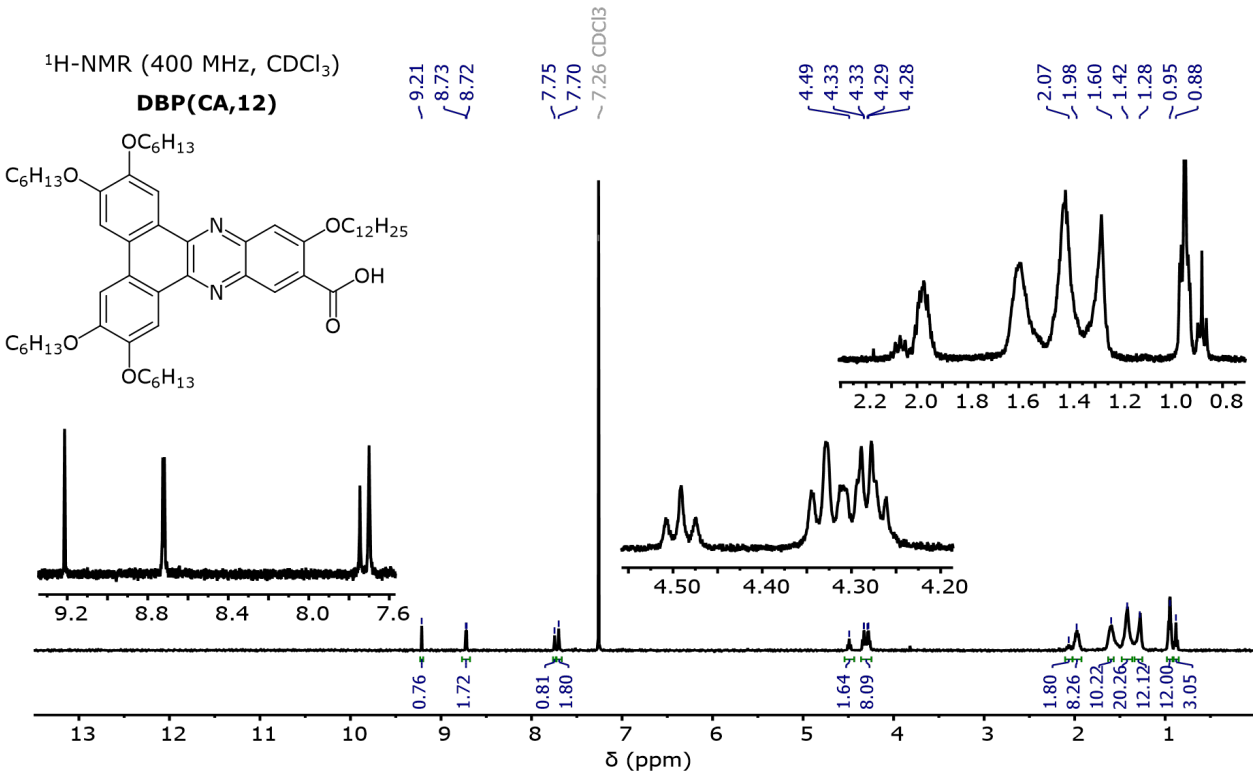


Figure S4. ^{13}C{^{1}H}-NMR spectrum of **DBP(Dod,12)**.



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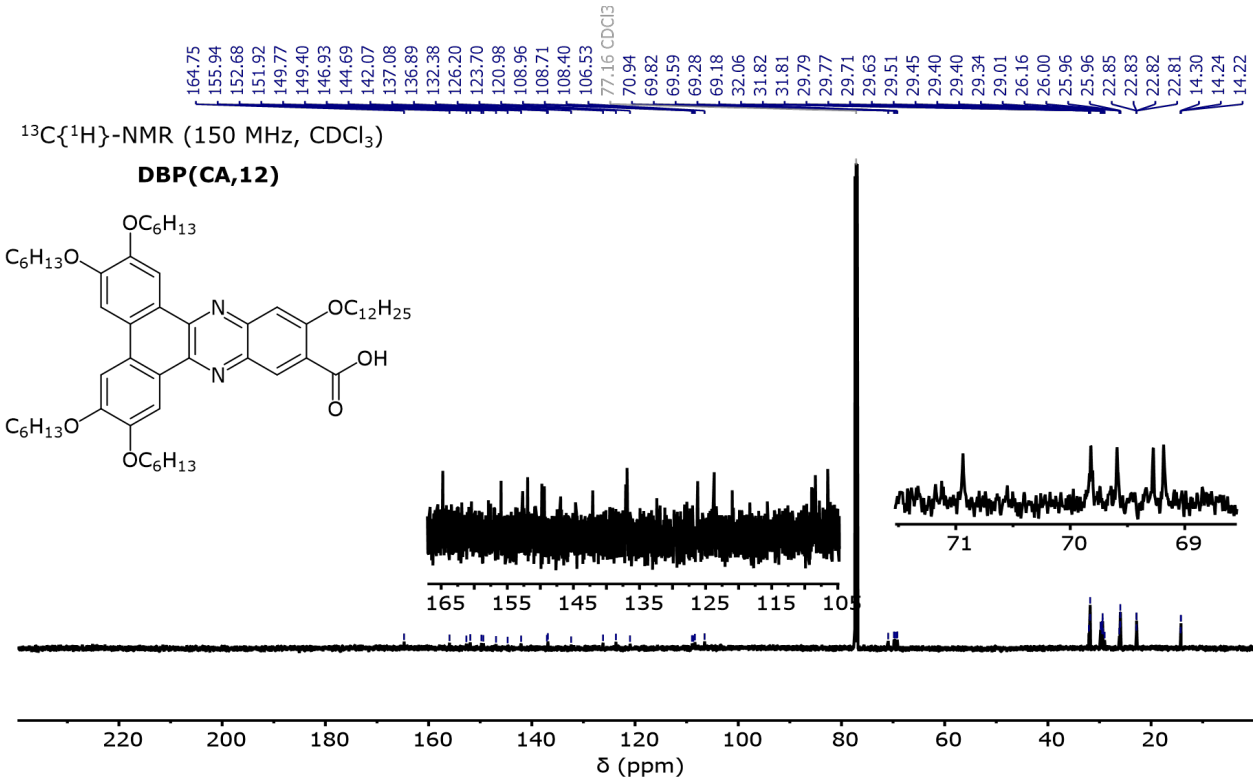

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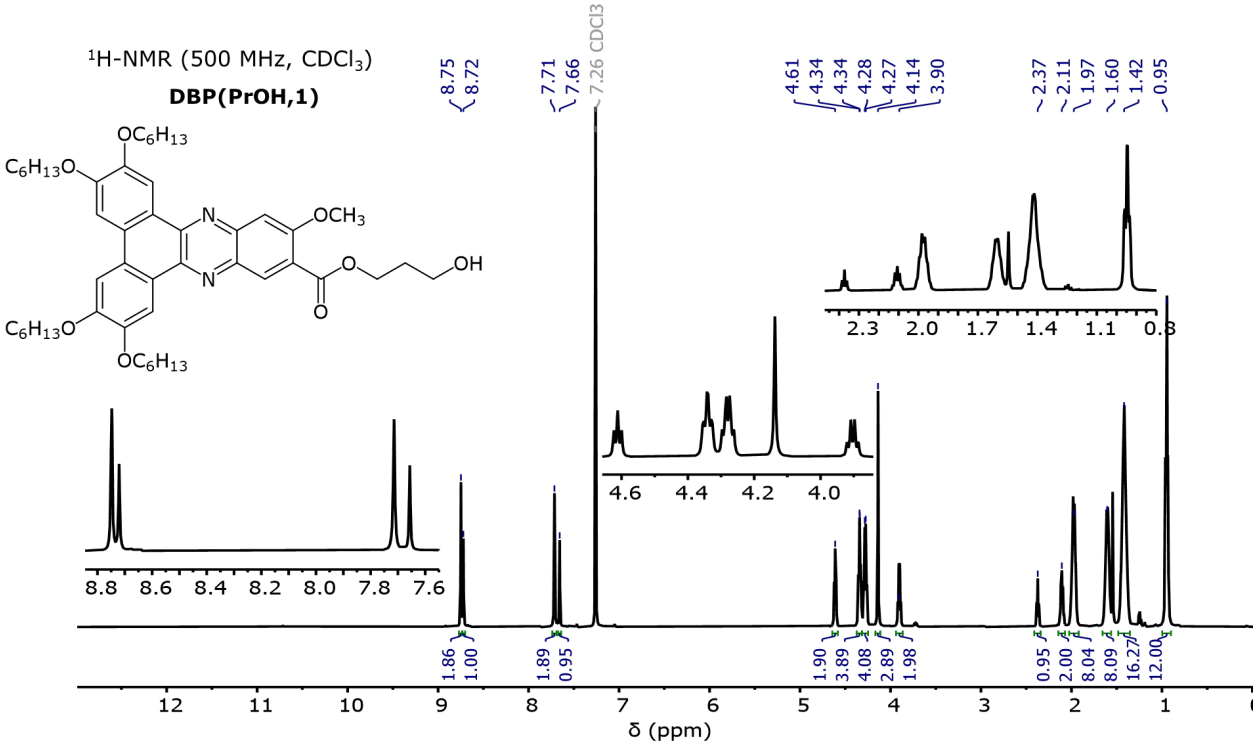

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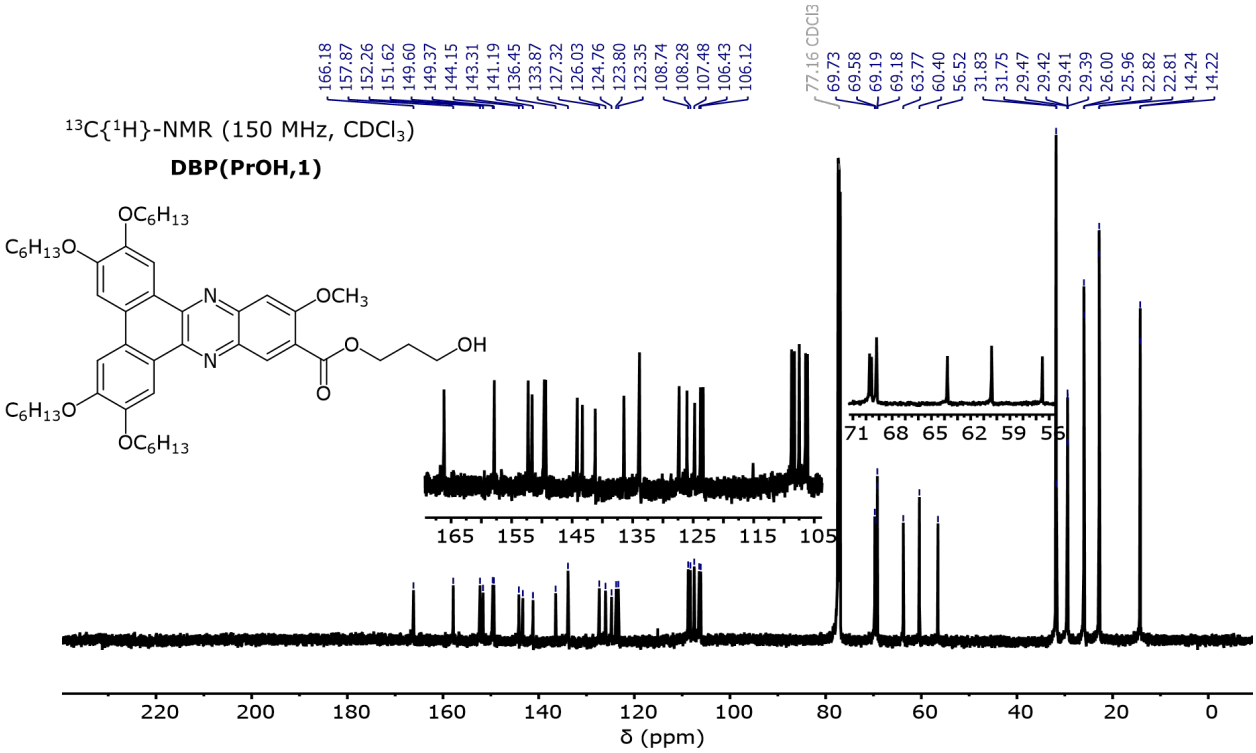

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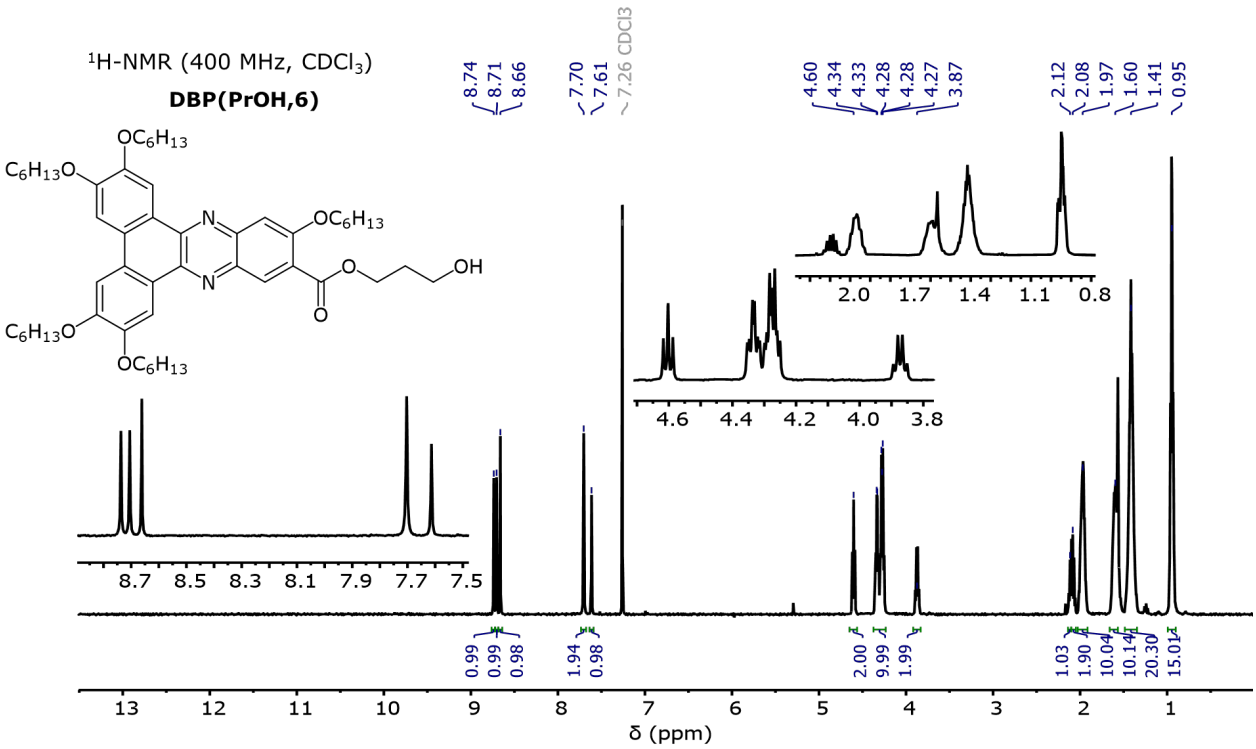

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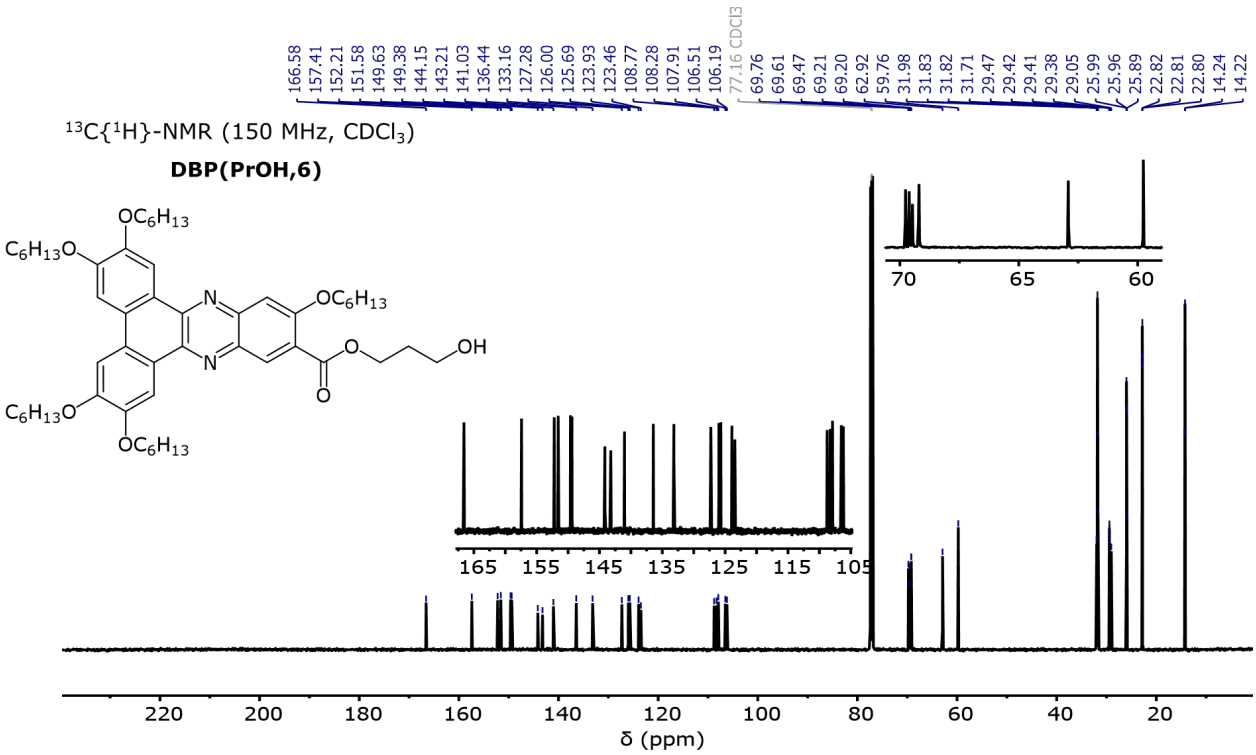
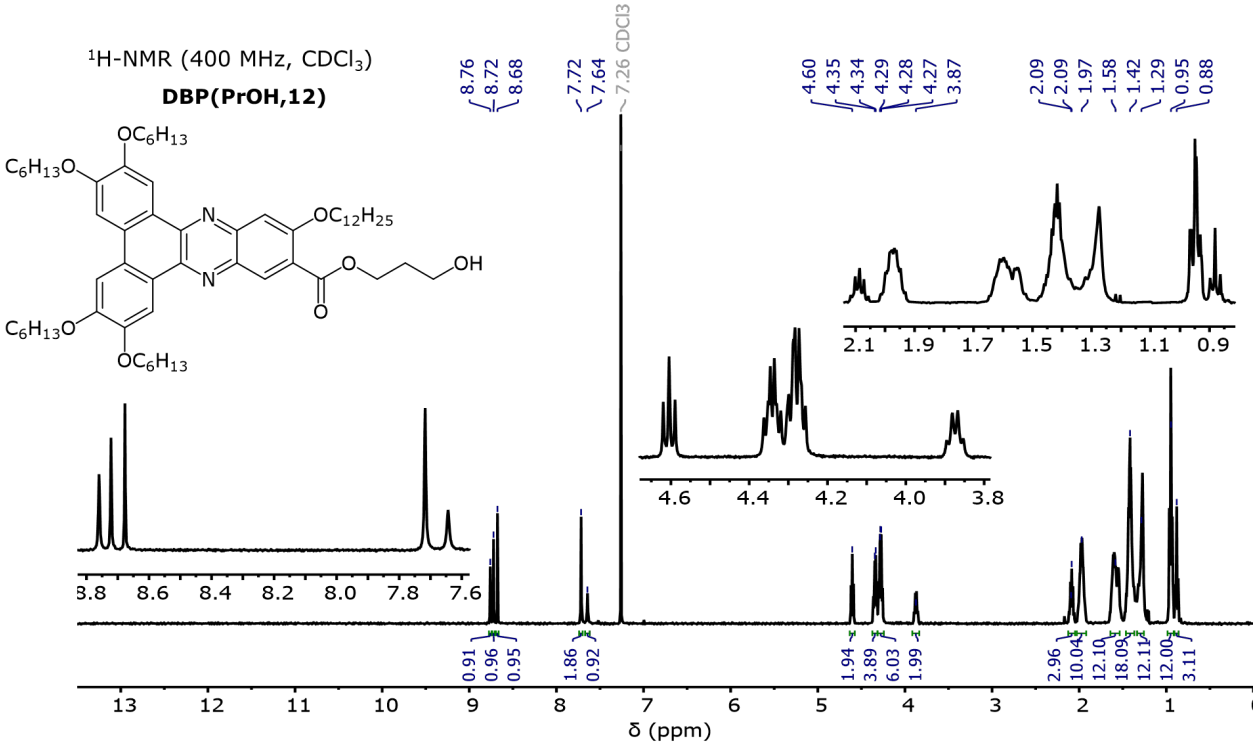


Figure S10. ^{13}C{^{1}H}-NMR spectrum of **DBP(PrOH,6)**.



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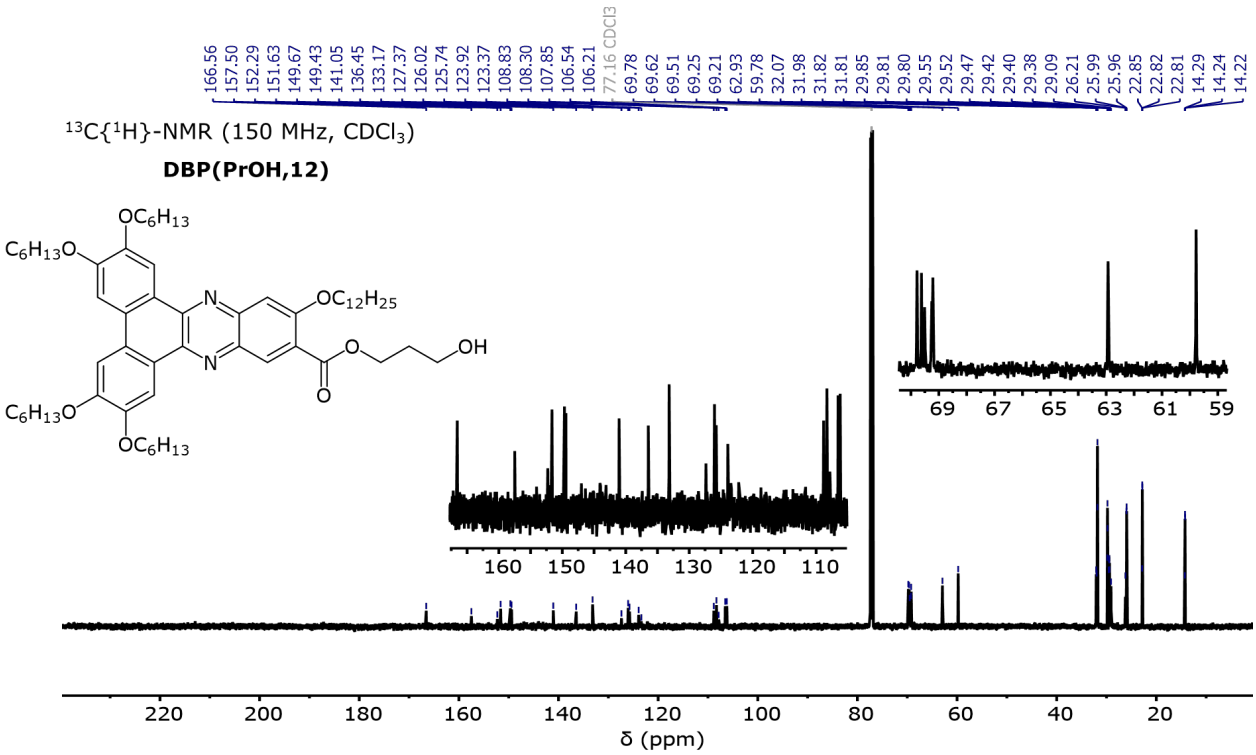
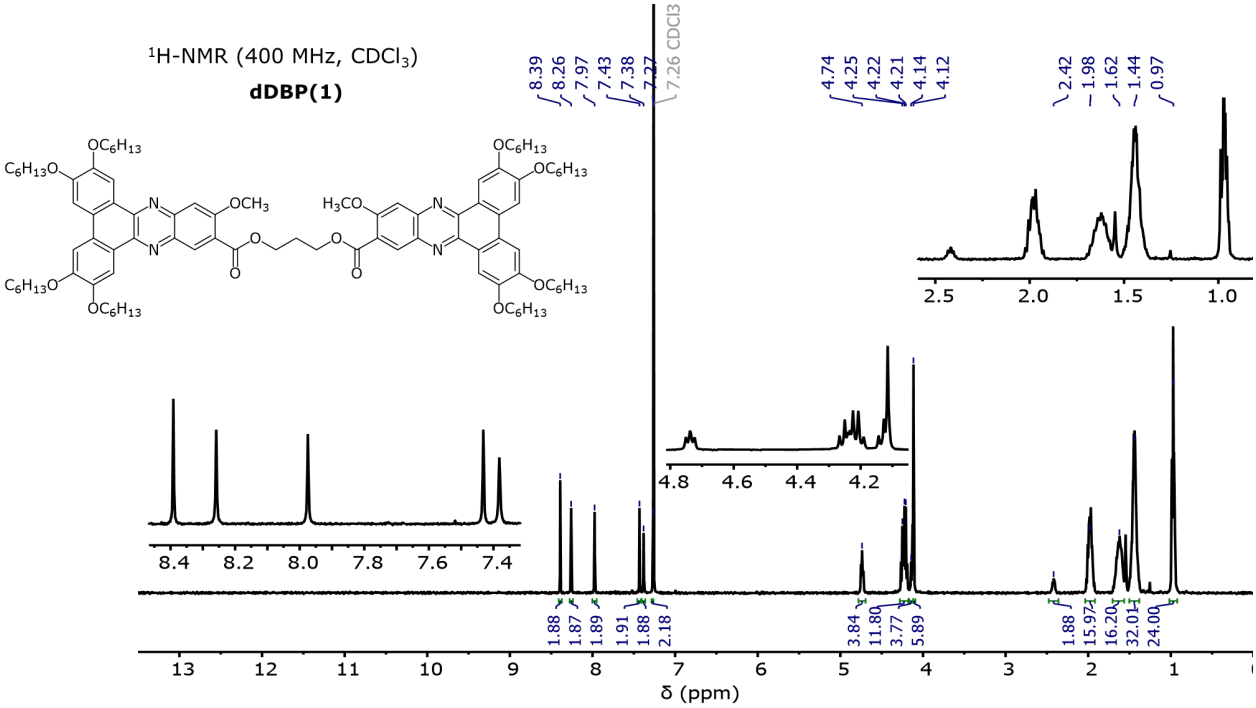


Figure S12. ^{13}C{^{1}H} NMR spectrum of **DBP(PrOH,12)**.



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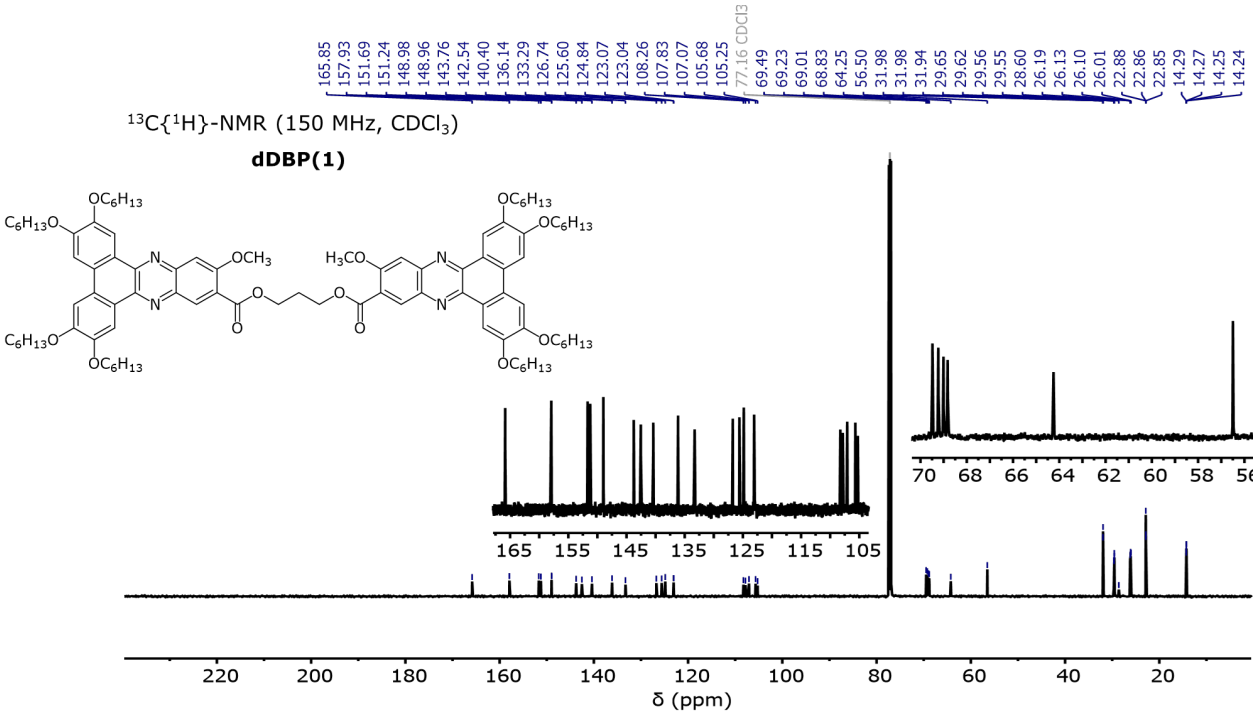
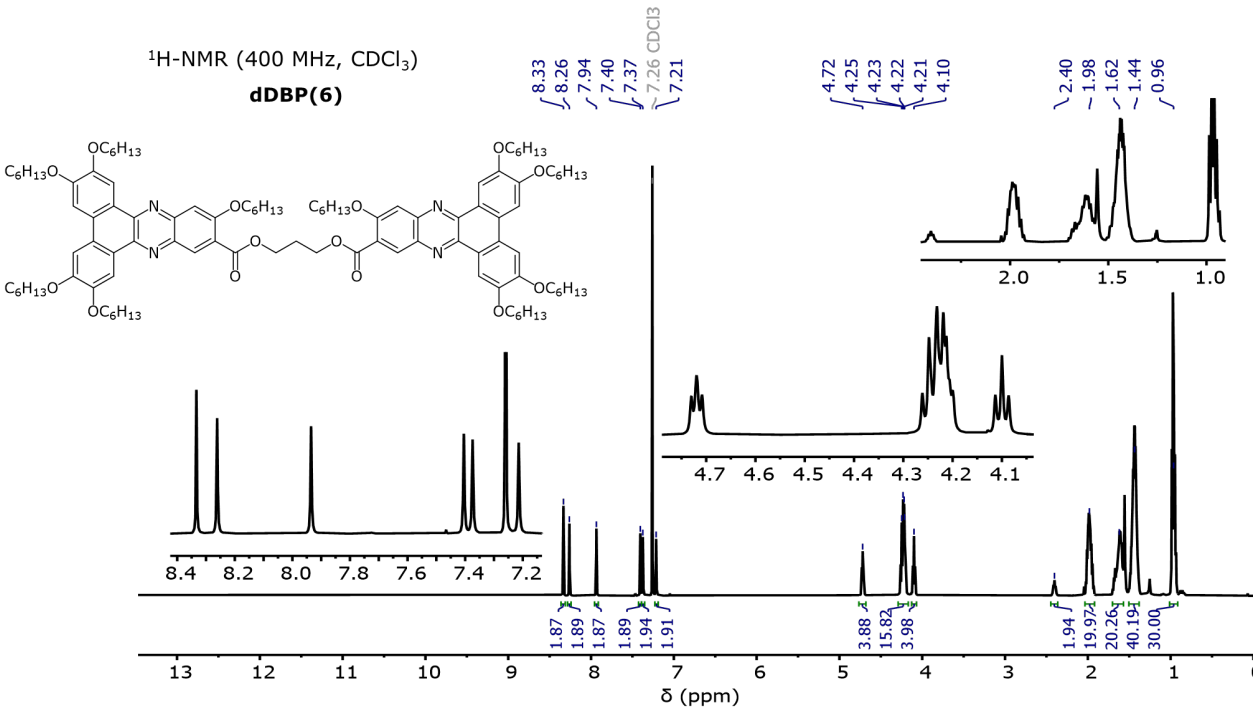


Figure S14. ^{13}C{^{1}H}-NMR spectrum of **dDBP(1)**.



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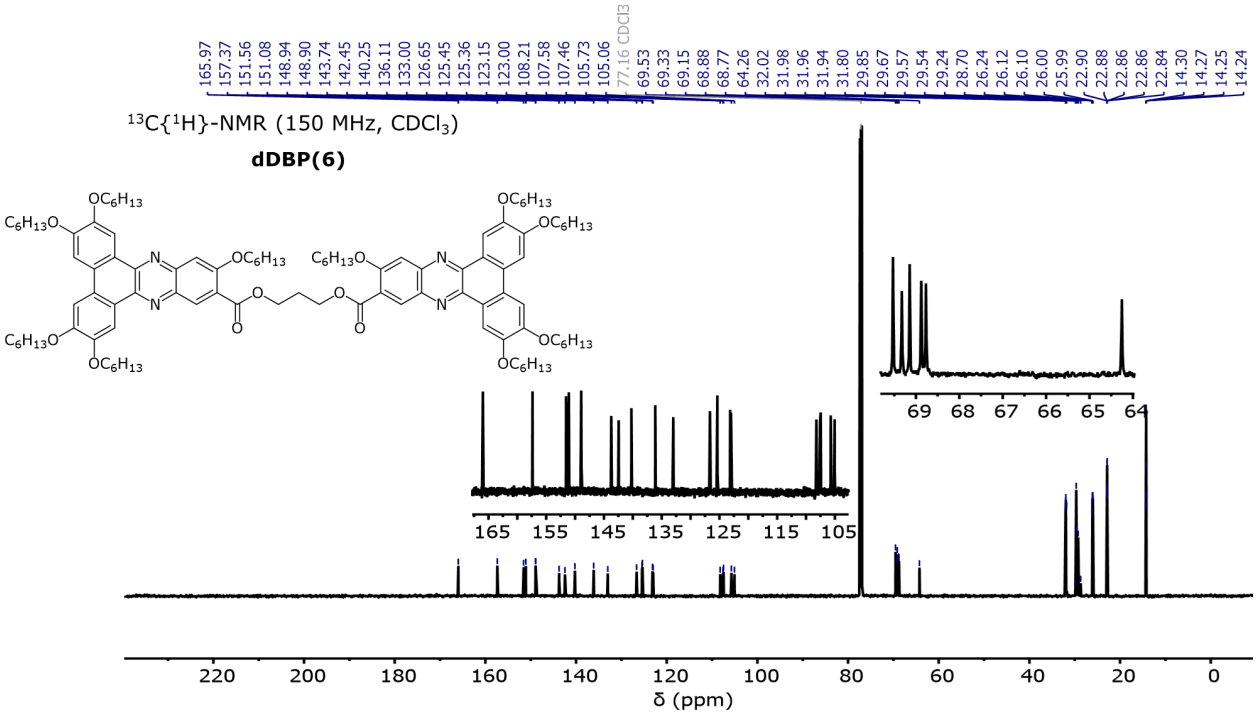

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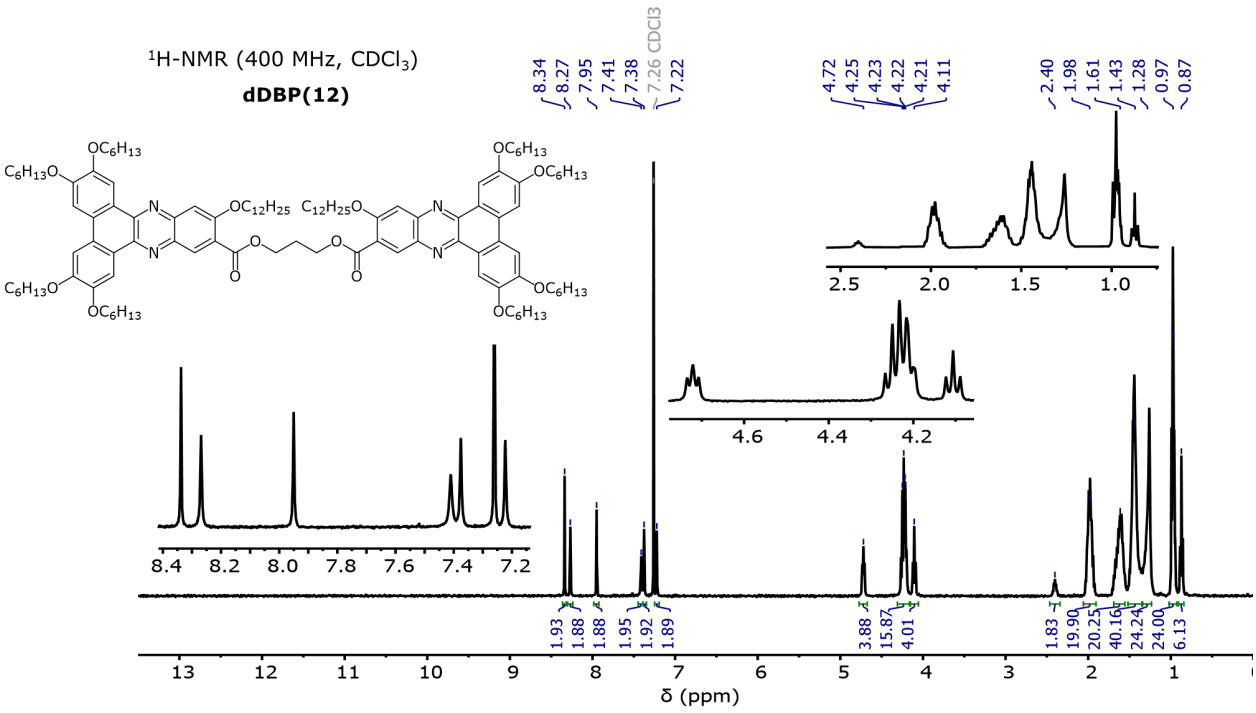

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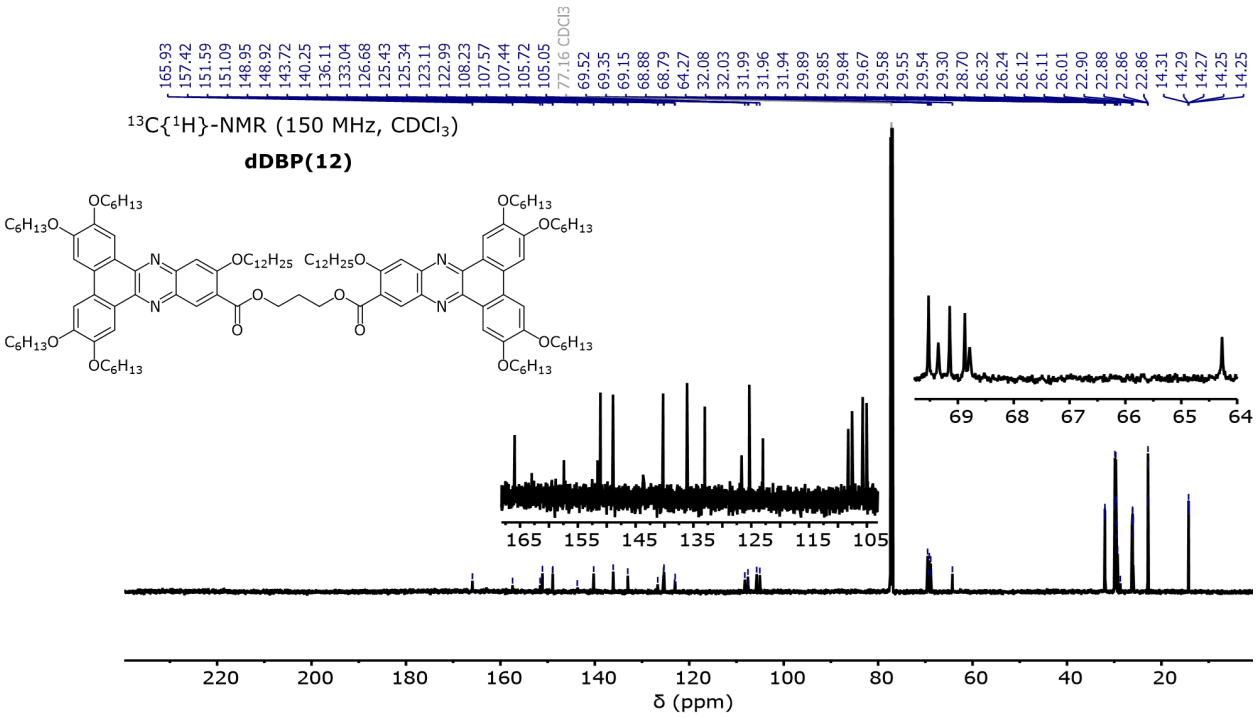

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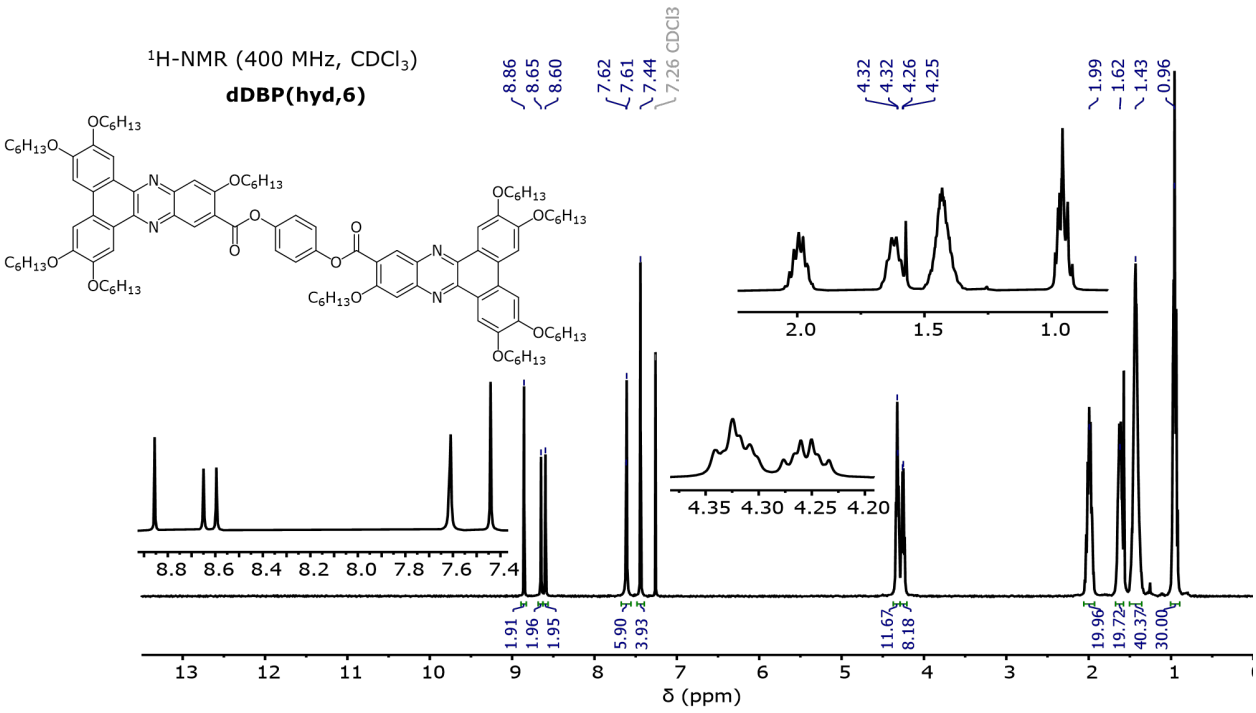


Figure S19. ^{1}H-NMR spectrum of **dDBP(hyd,6)**.

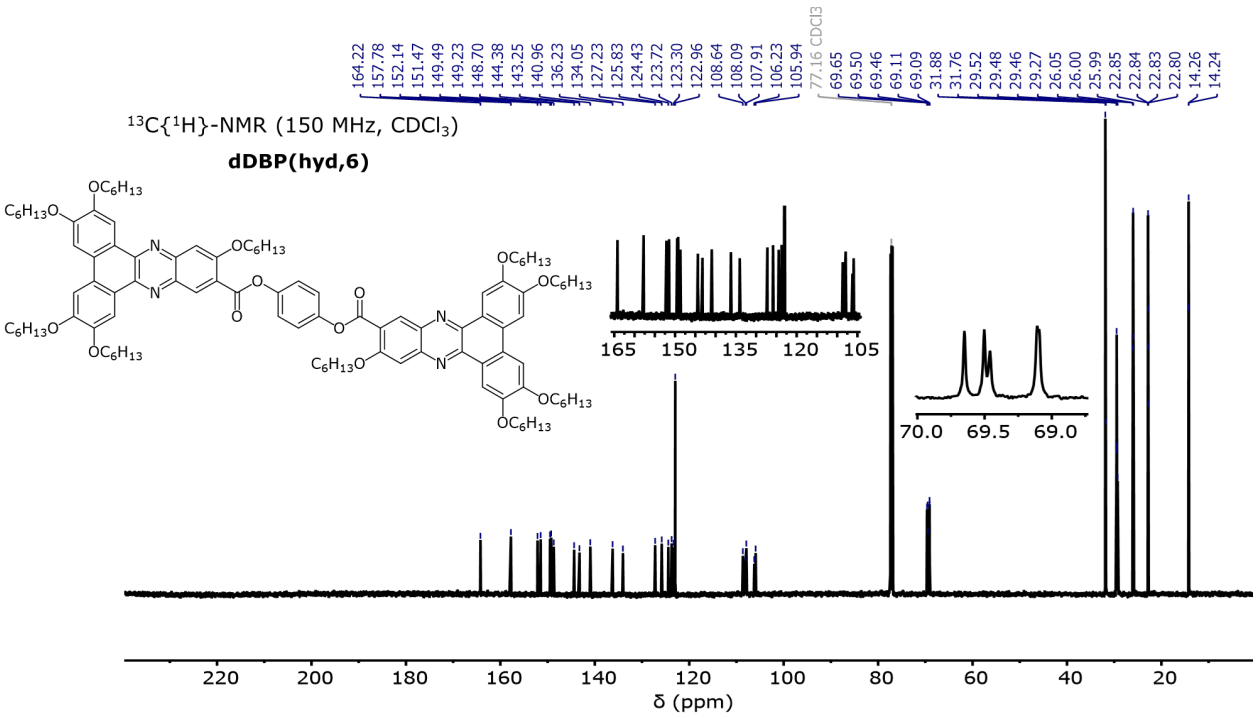


Figure S20. ^{13}C{^{1}H}-NMR spectrum of **dDBP(hyd,6)**.

2. Differential Scanning Calorimetry (DSC)

Phase transition temperatures and enthalpies were investigated using differential scanning calorimetry (DSC) on a DSC Q2000 instrument (TA Instruments) equipped with a refrigerated cooling system (TA Instruments, Refrigerated Cooling System 90). Heating and cooling measurements were performed at a rate of 10 °C/min. DSC thermograms of the first and second heating and cooling cycles for all compounds are shown.

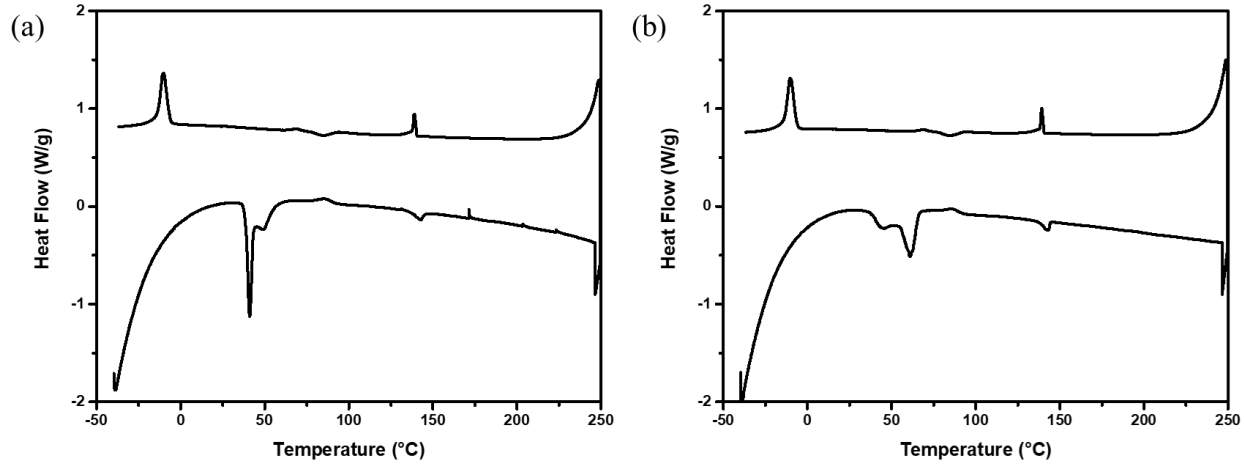
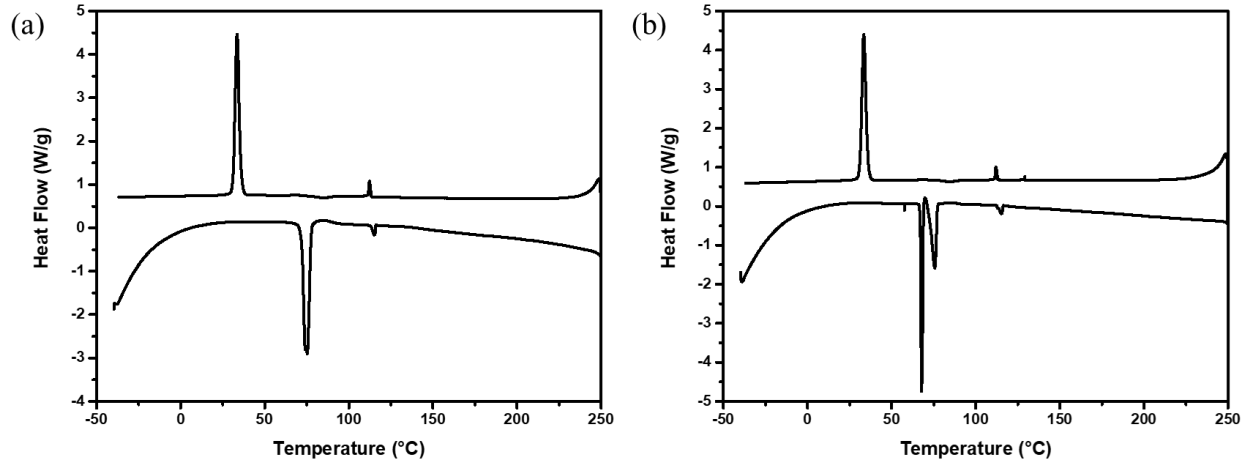


Figure S21. DSC thermograms of **DBP(Me,12)** for the (a) first and (b) second heating/cooling cycles.



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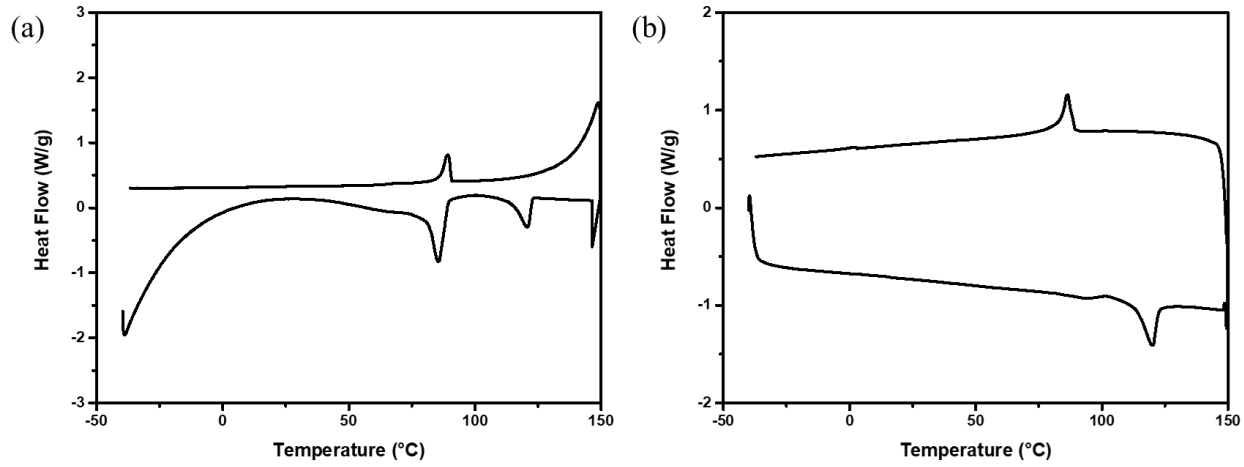
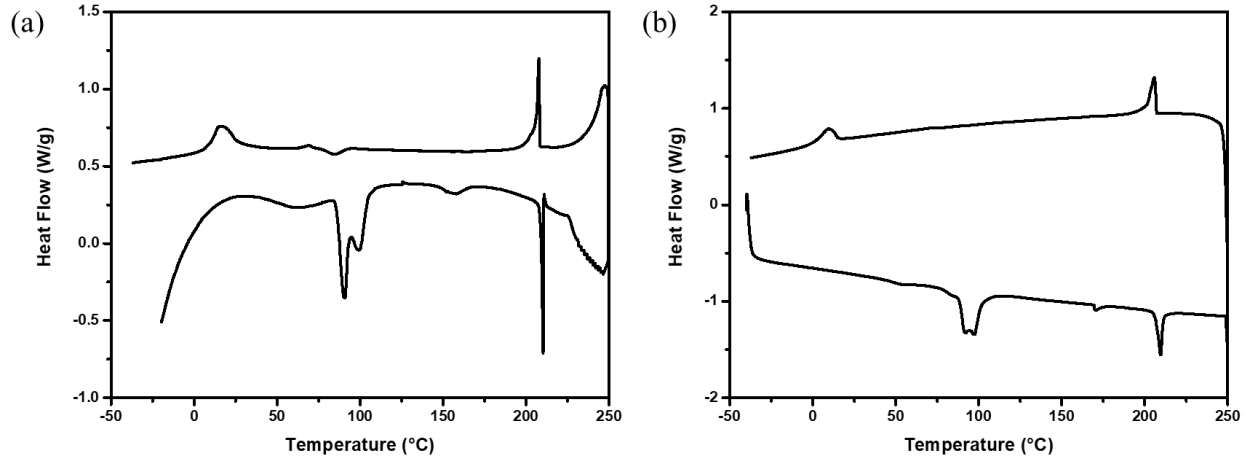


Figure S23. DSC thermograms of **DBP(CA,12)** for the (a) first and (b) second heating/cooling cycles.



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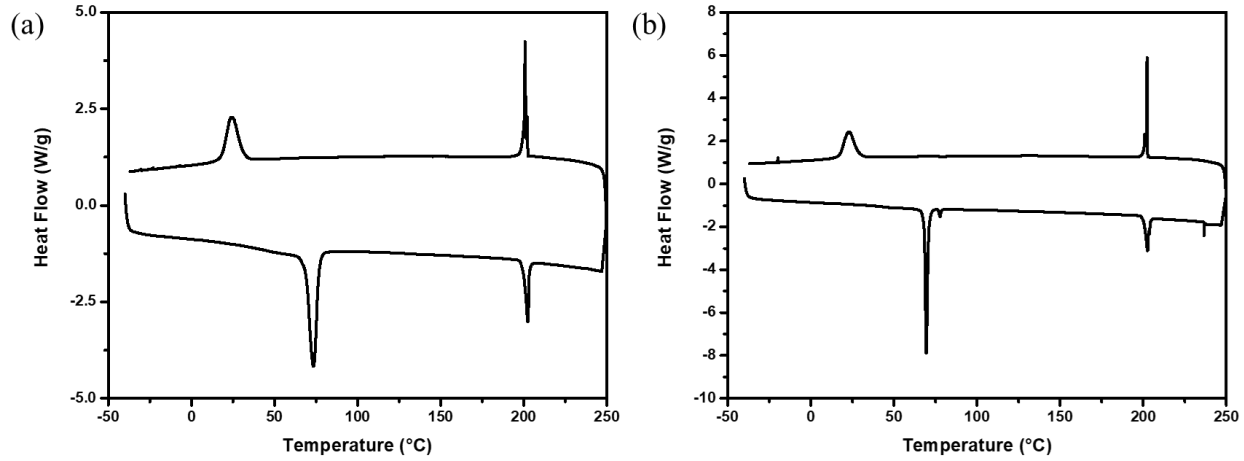


Figure S25. DSC thermograms of **DBP(PrOH,6)** for the (a) first and (b) second heating/cooling cycles.

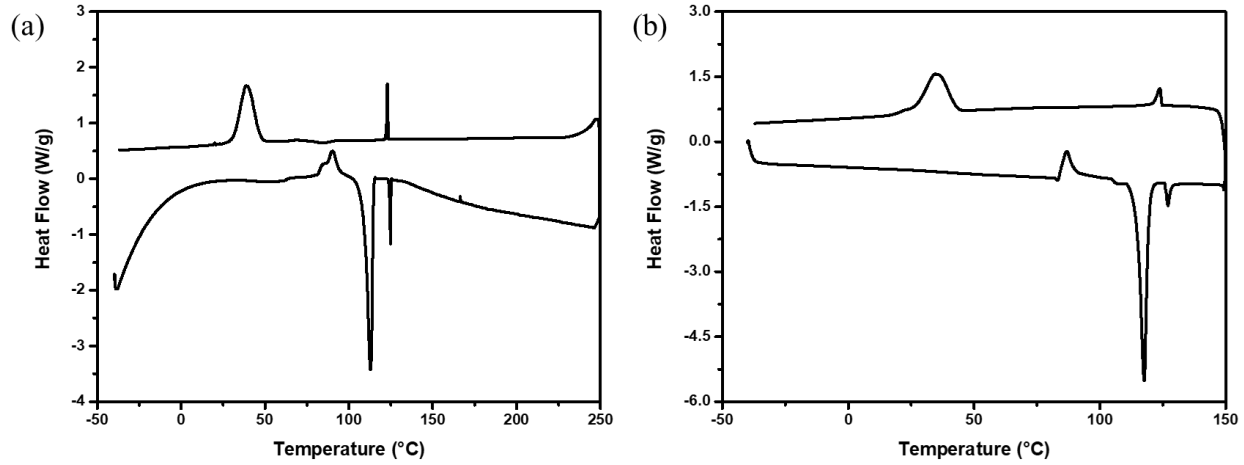


Figure S26. DSC thermograms of **DBP(PrOH,12)** for the (a) first and (b) second heating/cooling cycles.

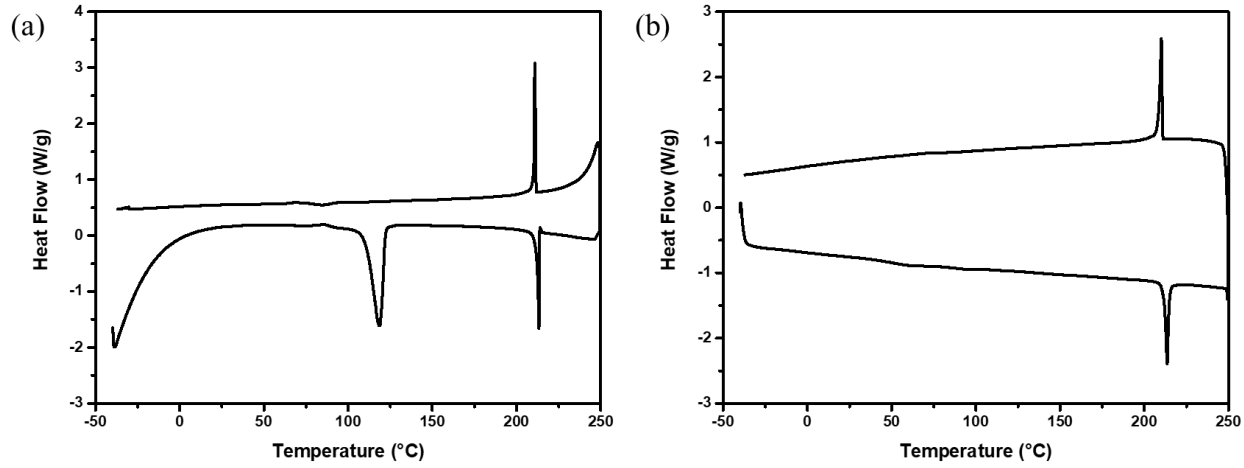


Figure S27. DSC thermograms of **dDBP(1)** for the (a) first and (b) second heating/cooling cycles.

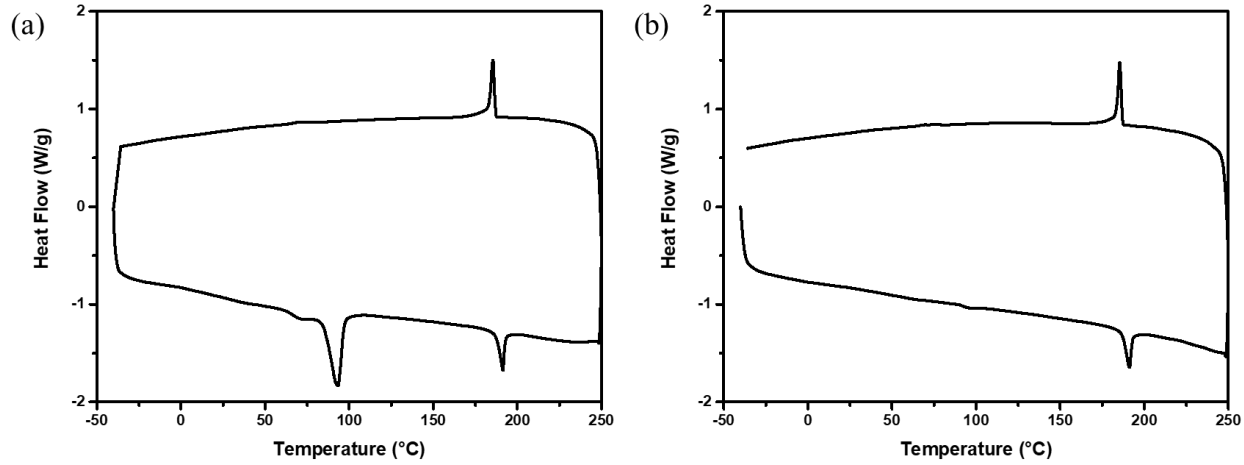


Figure S28. DSC thermograms of **dDBP(6)** for the (a) first and (b) second heating/cooling cycles.

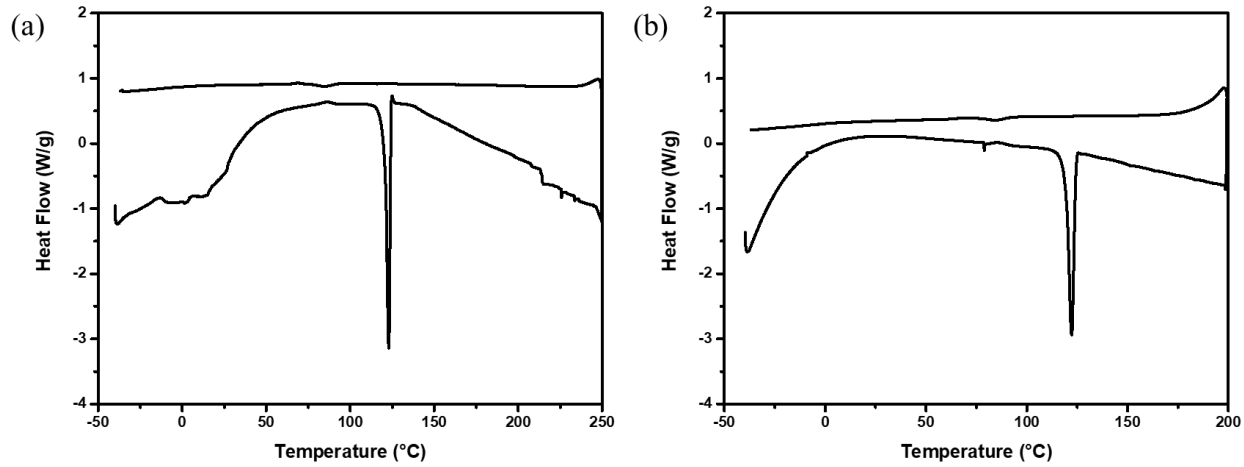


Figure S29. DSC thermograms of **dDBP(12)** for the (a) first and (b) second heating/cooling cycles.

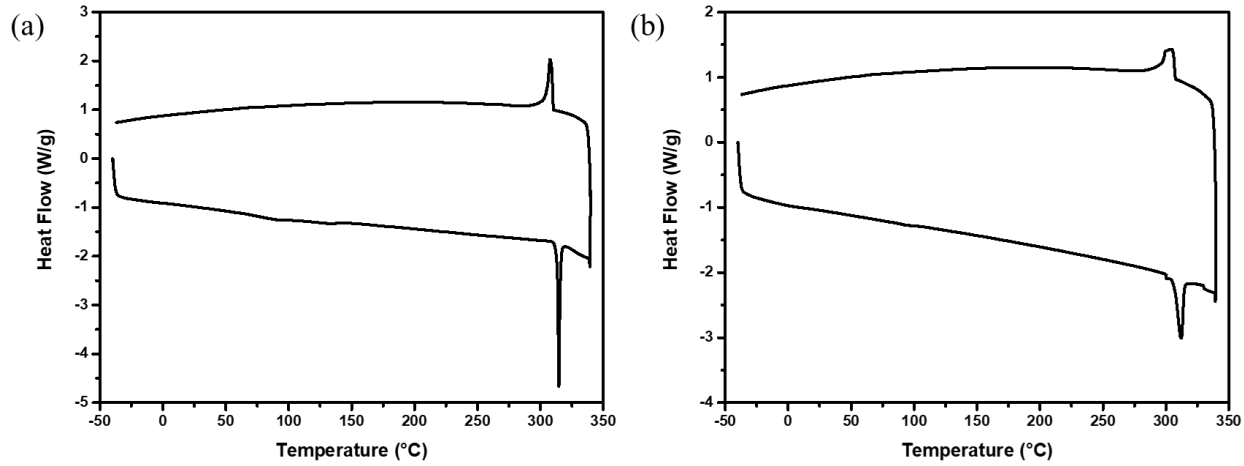


Figure S30. DSC thermograms of **dDBP(hyd,6)** for the (a) first and (b) second heating/cooling cycles.

Table S1. Phase behaviour of **dDBP(hyd,6)**.

Compound	Heating: Phase[a] T(°C) [ΔH (kJ·mol^{-1})][b] Phase[a]…	Cooling: Phase[a] T(°C) [ΔH (kJ·mol^{-1})][b] Phase[a]…
dDBP(hyd,6)	Col_h 314.8 [20.3] Iso	Iso [307.8 [-17.6] Col_h

[a]Phases identified by POM and vt-XRD expeimernts: Col_h = columnar hexagonal, Iso = isotropic liquid. [b]Transition temperatures and enthalpies were determined by DSC experiments (scan rate = 10 °C/min) on the first heating/cooling cycle.

3. Polarized Optical Microscopy (POM)

Texture and phase behaviour analyses were carried out using polarized optical microscopy (POM) on an Olympus BX50 microscope equipped with cross polarizers and a Linkam LTS350 heating stage. All images shown are of a size of ca. 920 x 1400 µm, unless otherwise specified.

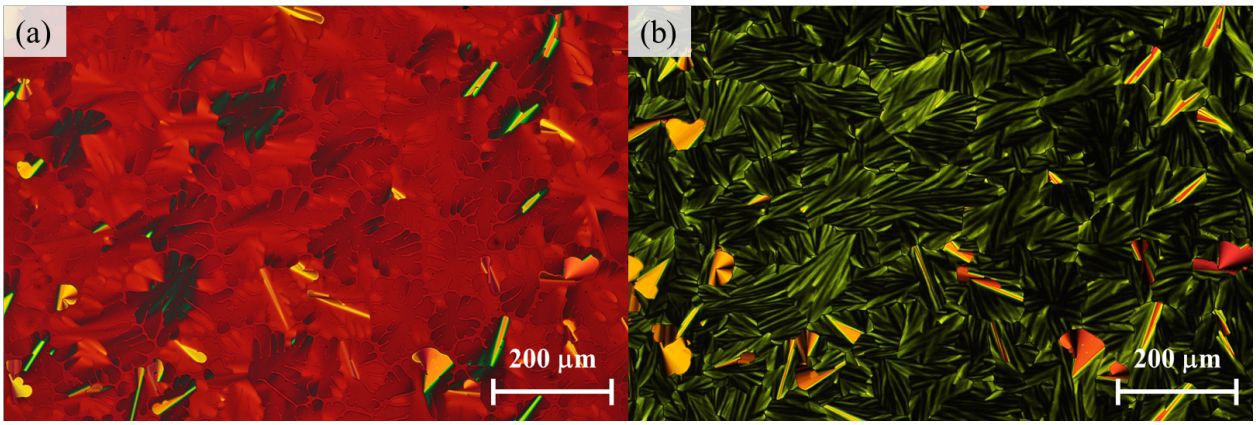


Figure S31. Polarized optical micrographs of **DBP(Me,12)** showing dendritic textures with sixfold symmetry of the Col_h phase at 139 °C. Image (b) shows the sample after being cooled to room temperature. Image (a) was taken with a 530 nm quarter wavelength retardation plate.

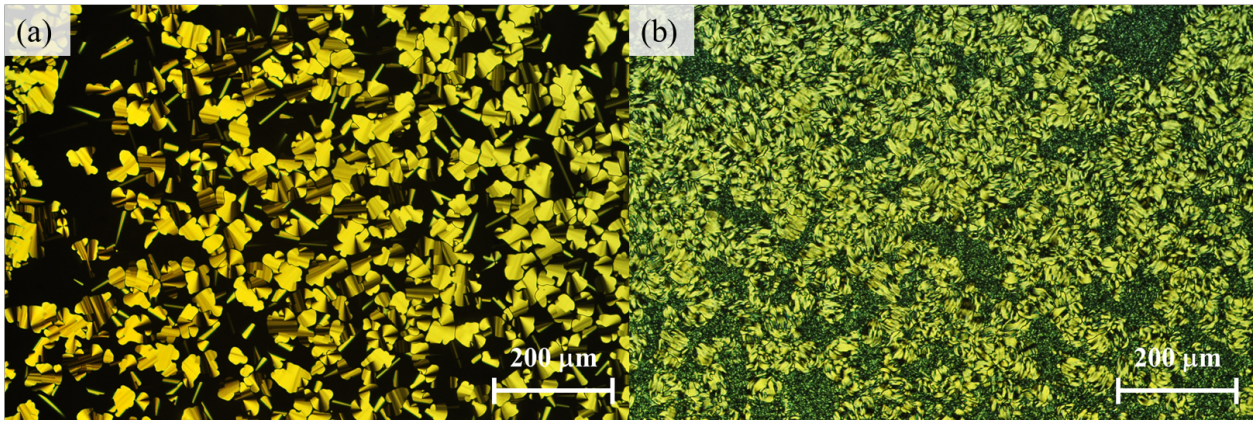


Figure S32. Polarized optical micrographs of **DBP(Dod,12)** showing (a) fan-shaped textures of the Col_h phase at 109 °C and (b) the crystalline phase at room temperature.

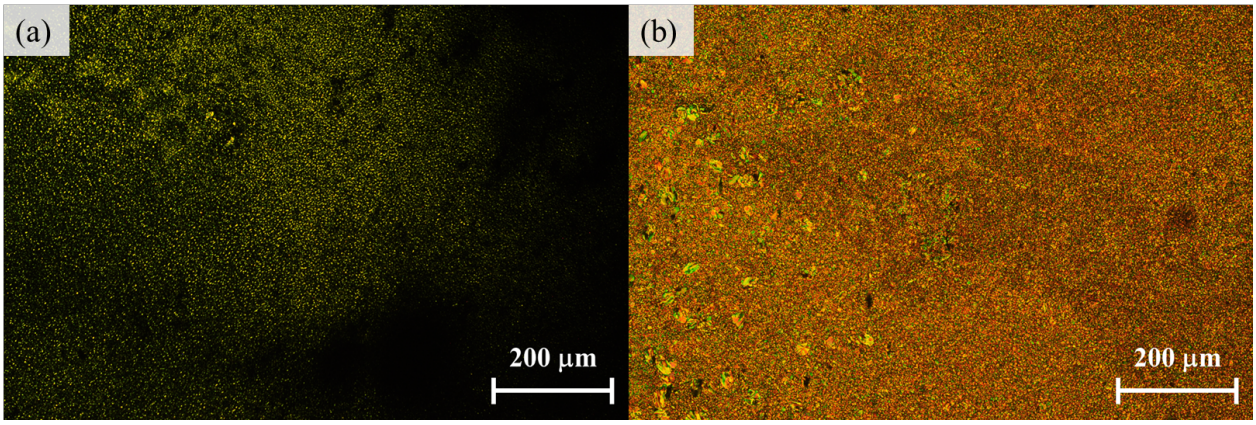


Figure S33. Polarized optical micrographs of **DBP(CA,12)** showing grain-like textures of the crystalline phase at (a) 104 °C and (b) room temperature.

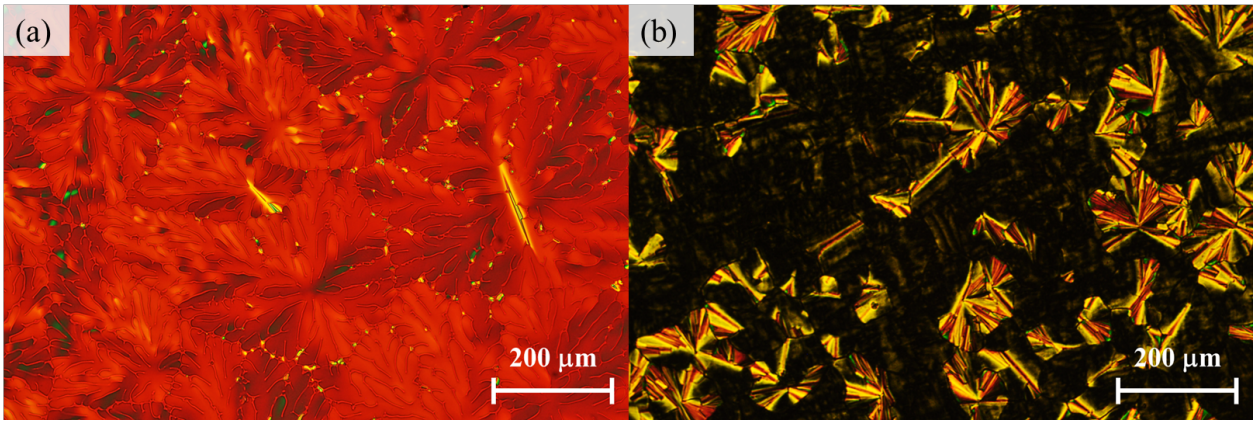


Figure S34. Polarized optical micrographs of **DBP(PrOH,1)** showing (a) dendritic textures with sixfold symmetry of the Col_h phase at 207 °C. Image (b) shows the sample after being cooled to room temperature. Image (a) was taken with a 530 nm quarter wavelength retardation plate.

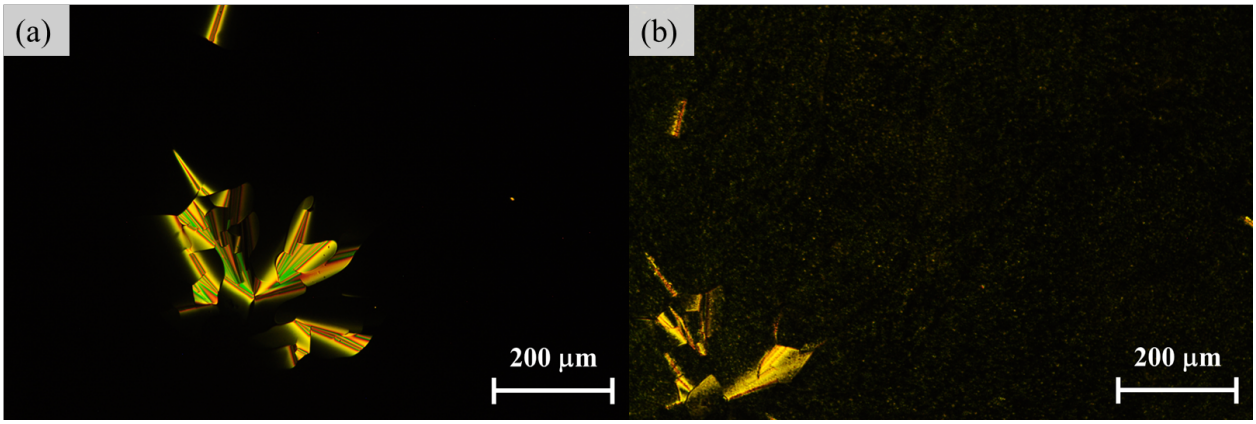


Figure S35. Polarized optical micrographs of **DBP(PrOH,6)** showing (a) fan-shaped textures of the Col_h phase at 199 °C and (b) grain-like textures of the crystalline phase at room temperature.

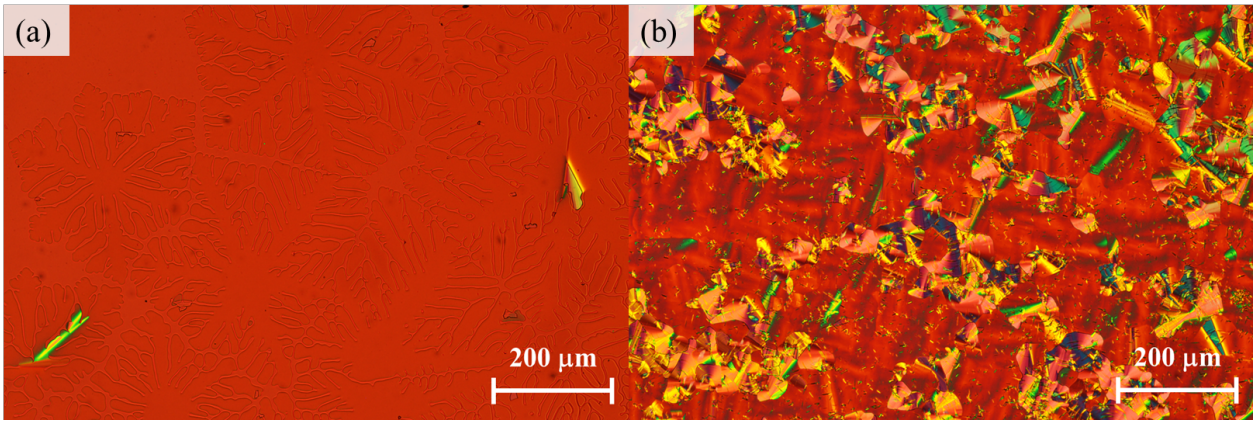


Figure S36. Polarized optical micrographs of **DBP(PrOH,12)** showing (a) dendritic textures with sixfold symmetry of the Col_h phase at 123 °C and (b) the emergence of needle-like textures of the crystalline phase at 52 °C. Both images were taken with a 530 nm quarter wavelength retardation plate.

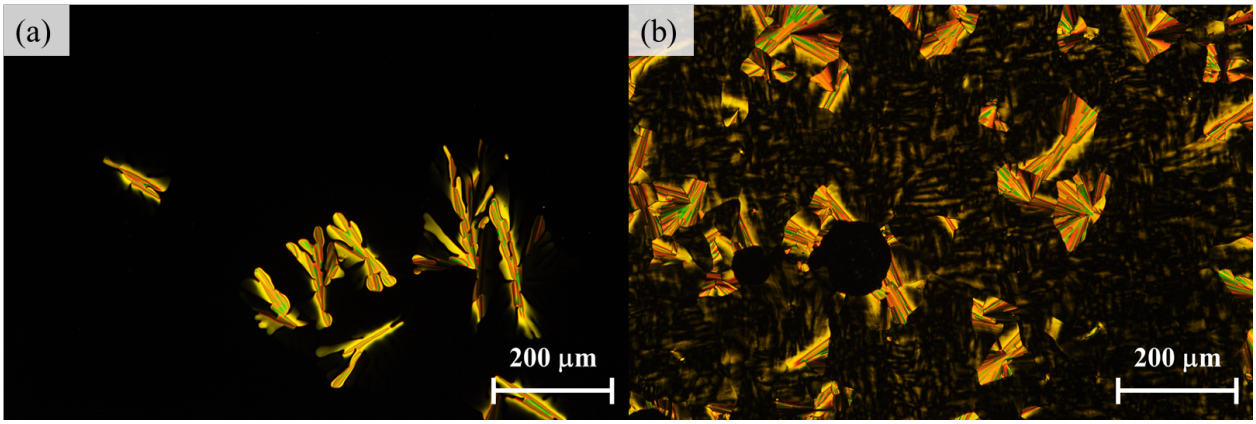


Figure S37. Polarized optical micrographs of **dDBP(1)** showing (a) dendritic textures with sixfold symmetry of the Col_h phase at 211 °C. Image (b) shows the retention of Col_h ordering after the sample is cooled to room temperature.

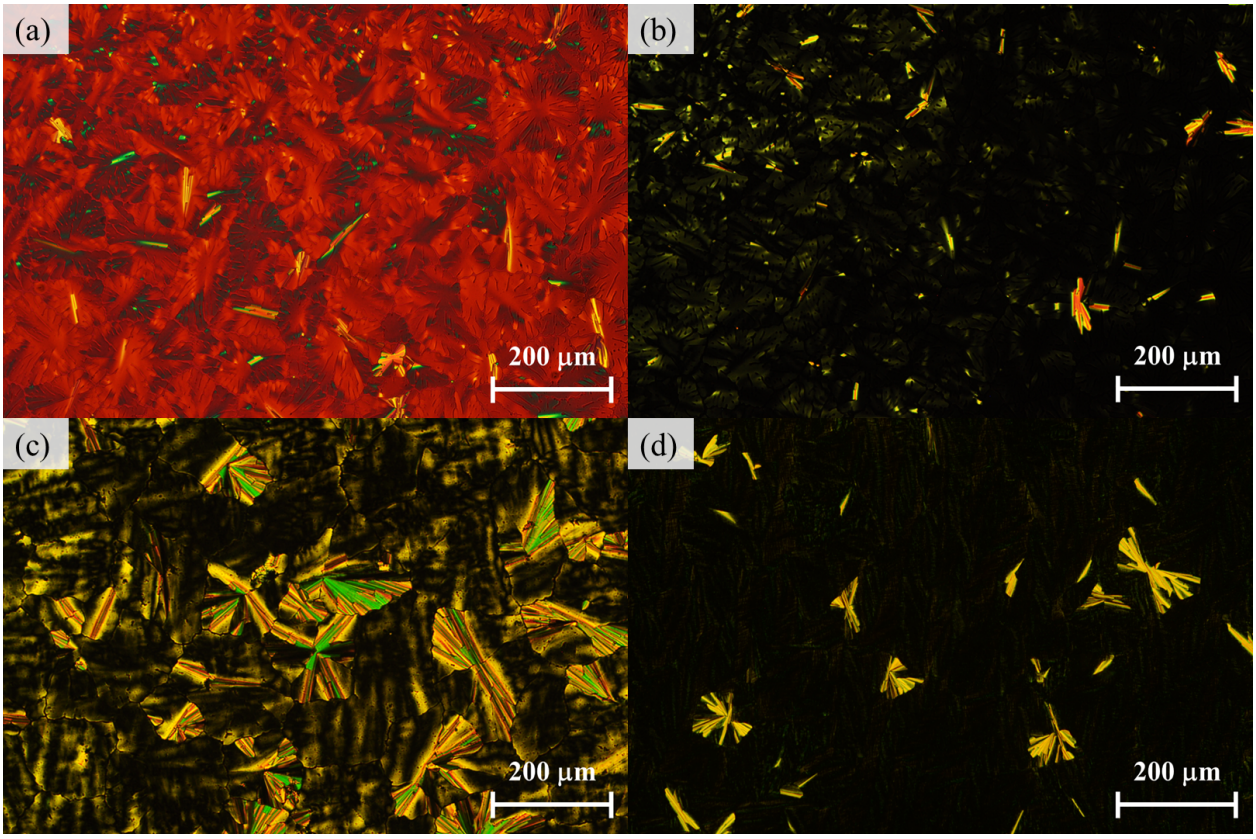


Figure S38. Polarized optical micrographs of **dDBP(6)** showing (a-b) dendritic textures of the Col_h phase at 186 °C in the same plane of view. Image (a) was taken with a 530 nm quarter wavelength retardation plate. Image (c) shows retention of Col_h ordering at room temperature after 30 minutes. Image (d) shows the sample at room temperature after 5 years.

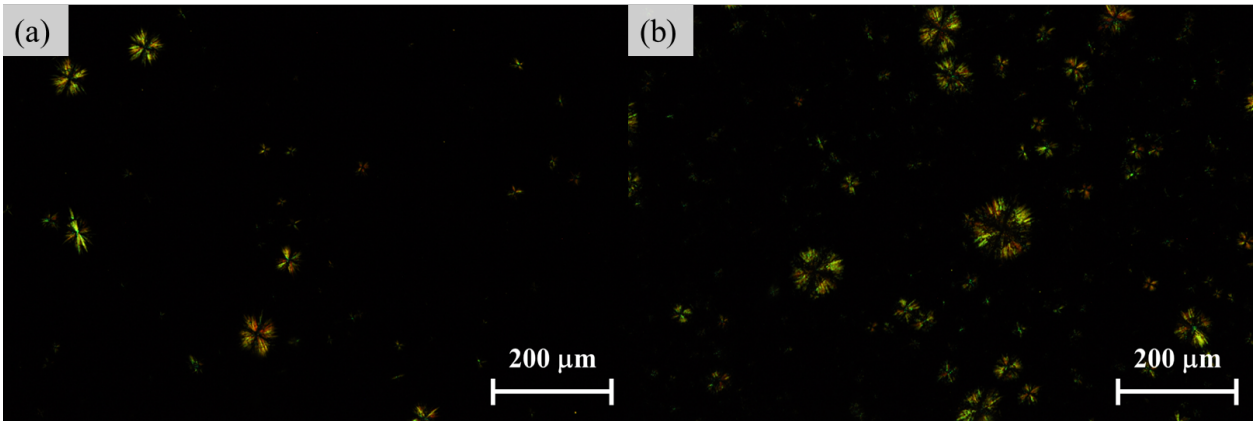


Figure S39. Polarized optical micrographs of **dDBP(12)** showing spherulitic textures of the crystalline phase at (a) 77 °C and (b) room temperature.

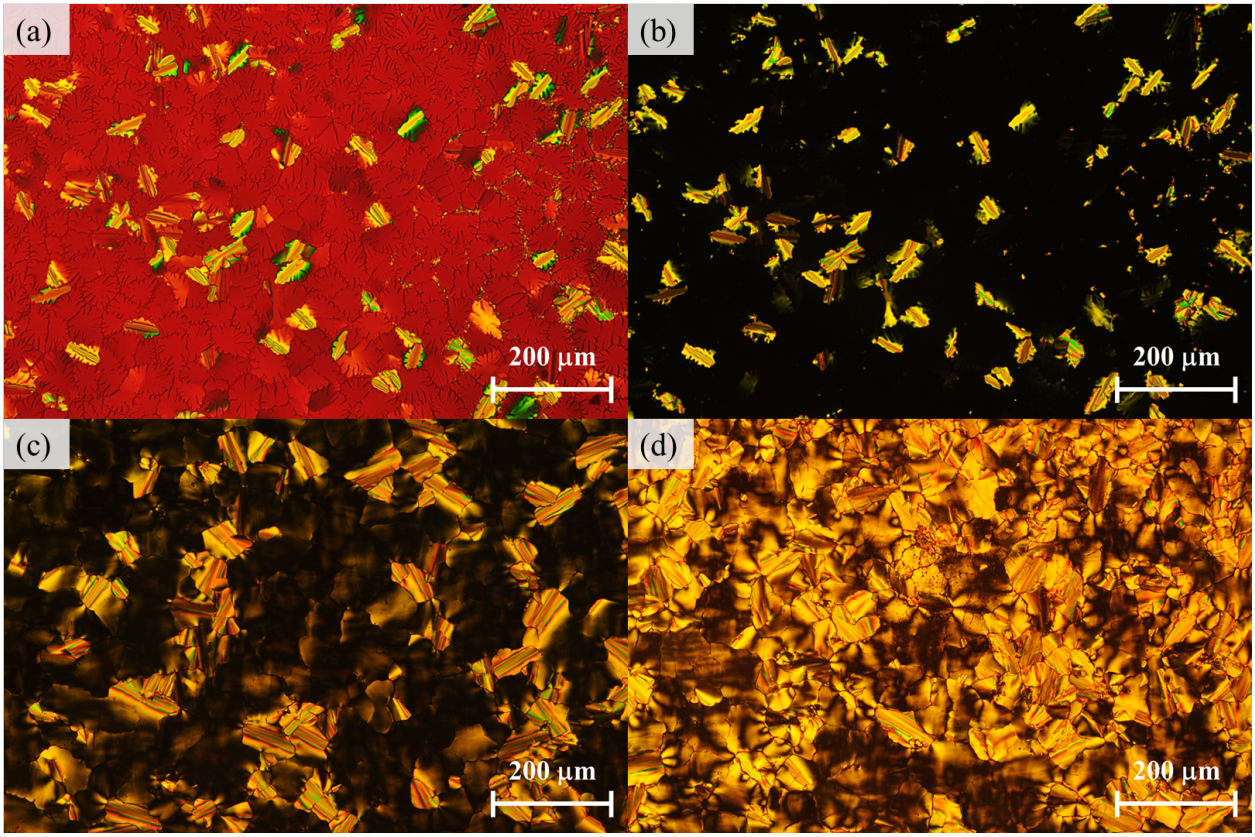


Figure S40. Polarized optical micrographs of **dDBP(hyd,6)** showing (a-b) dendritic textures of the Col_h phase at 306 °C in the same plane of view. Image (a) was taken with a 530 nm quarter wavelength retardation plate. Images (c) and (d) show retention of Col_h ordering at room temperature after 30 minutes and 10 months, respectively.

4. Variable Temperature X-ray Diffraction (VT-XRD)

Variable temperature X-ray scattering experiments were conducted on an X-ray diffractometer (Rigaku R-Axis Rapid) equipped with an in-house built temperature controller,[1] except for **dDBP(hyd,6)**, which was measured on a SAXSLAB Ganesha 300 XL small angle X-ray scattering (SAXS) system. Samples of **dDBP(hyd,6)** were loaded into thin-walled quartz capillary tubes with a 1.5 mm outer diameter (Charles Supper Company) and were mounted in a Linkam T95-PE heating stage. Room temperature XRD measurements were performed on the SAXS system in which the glass capillaries used for the variable temperature measurements were mounted onto a SAXSLAB 8·8, 4 mm Mask ambient sample plate.

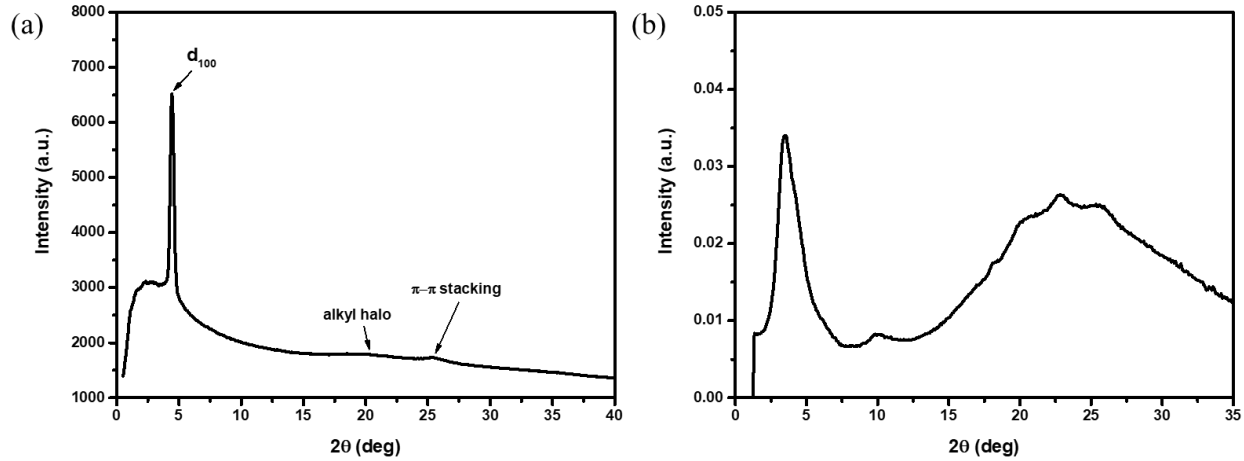


Figure S41. X-ray diffractograms of **DBP(Me,12)** at (a) 104 °C on the Rigaku instrument and (b) room temperature on the SAXS instrument.

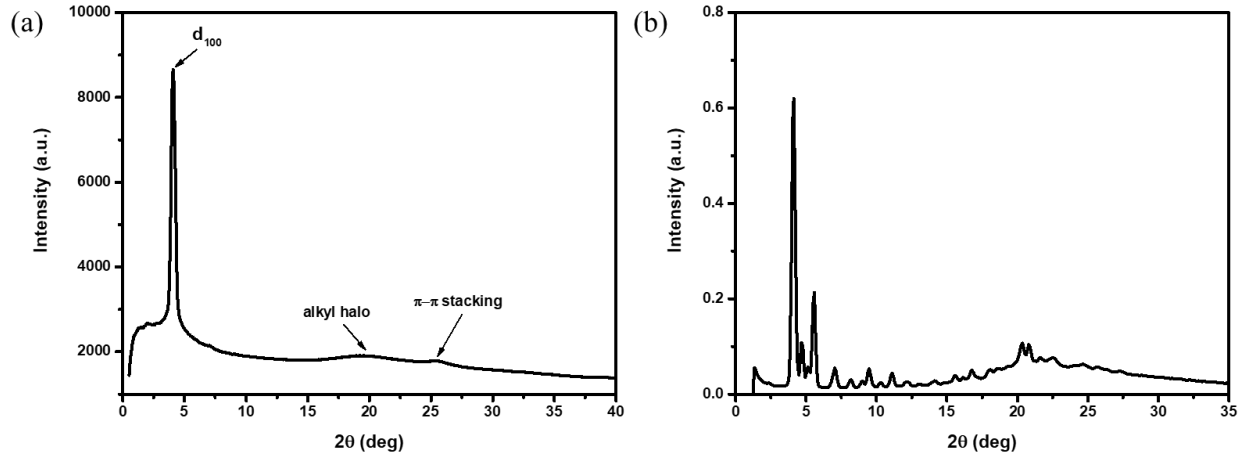


Figure S42. X-ray diffractograms of **DBP(Dod,12)** at (a) 95 °C on the Rigaku instrument and (b) room temperature on the SAXS instrument.

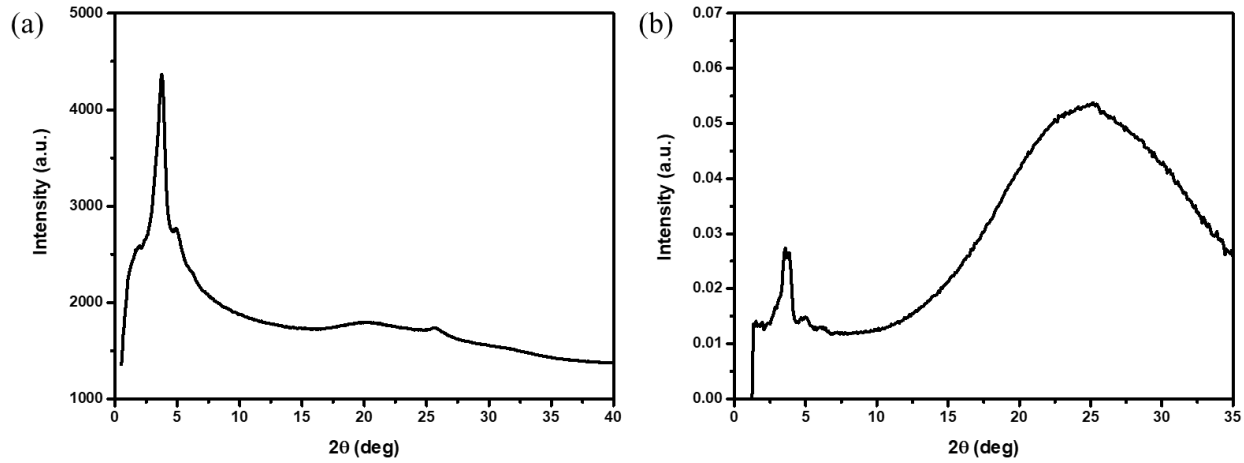


Figure S43. X-ray diffractograms of **DBP(CA,12)** at room temperature on (a) the Rigaku instrument and (b) the SAXS instrument.

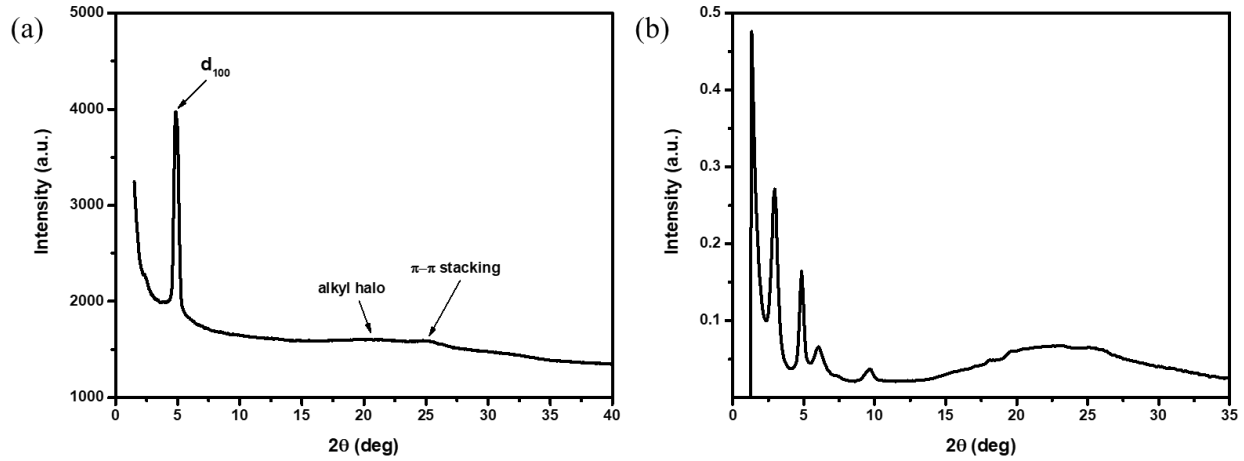


Figure S44. X-ray diffractograms of **DBP(PrOH,1)** at (a) 178 °C on the Rigaku instrument and (b) room temperature on the SAXS instrument.

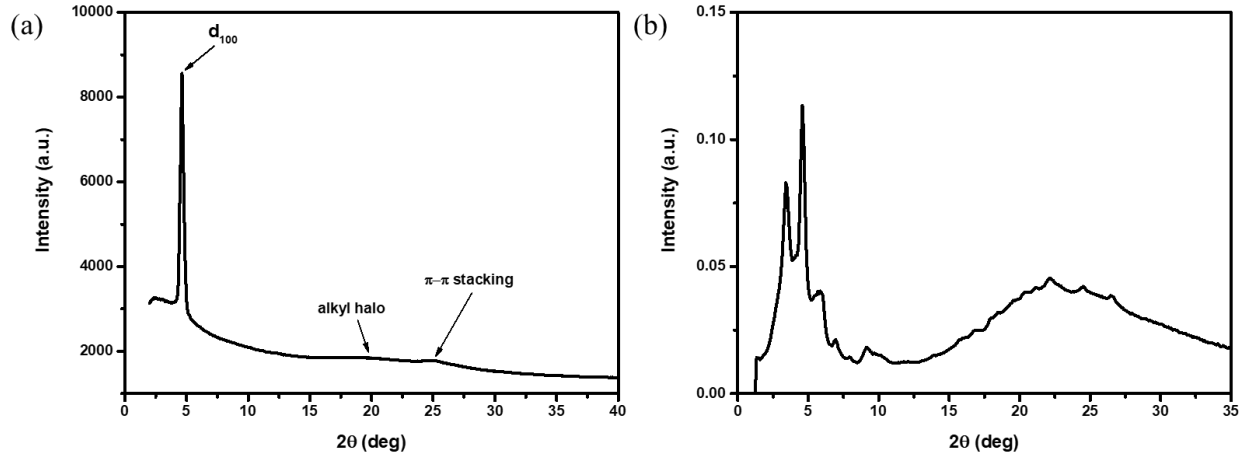


Figure S45. X-ray diffractograms of **DBP(PrOH,6)** at (a) 188 °C on the Rigaku instrument and (b) room temperature on the SAXS instrument.

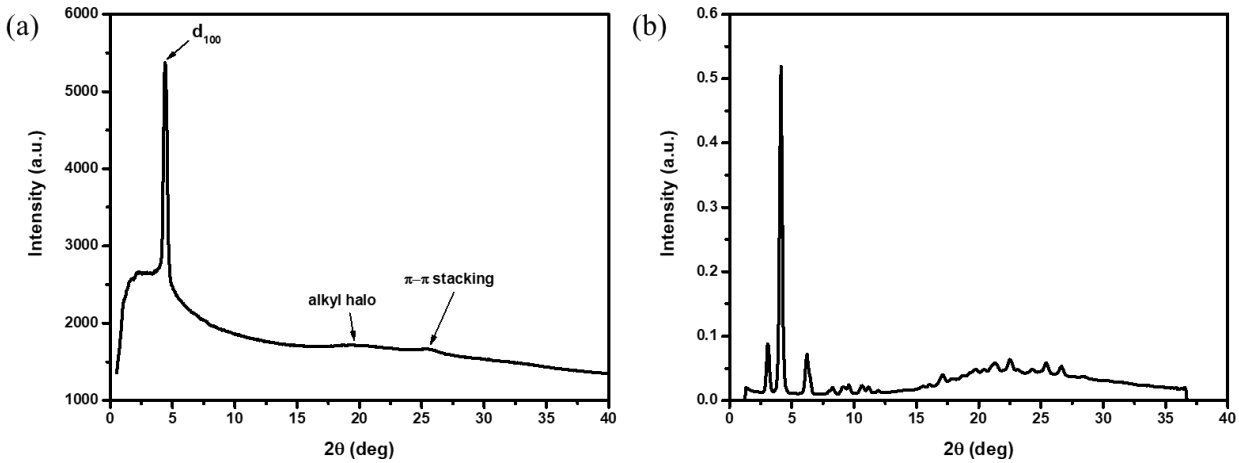


Figure S46. X-ray diffractograms of **DBP(PrOH,12)** at (a) 106 °C on the Rigaku instrument and (b) room temperature on the SAXS instrument.

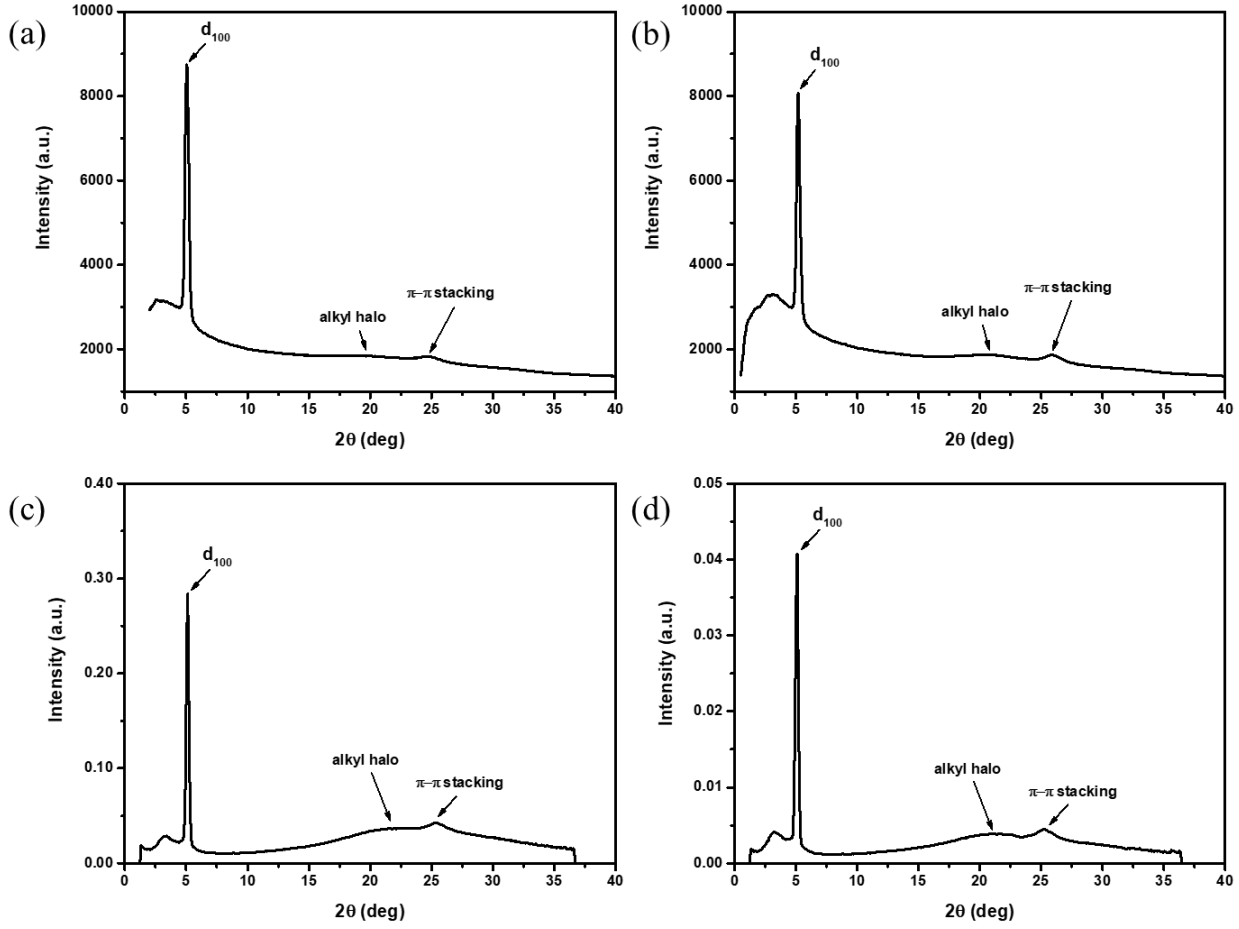


Figure S47. X-ray diffractograms of **dDBP(1)** at (a) 193 °C and (b) room temperature on the Rigaku instrument, and (c) 2 years and (d) 5 years at room temperature on the SAXS instrument.

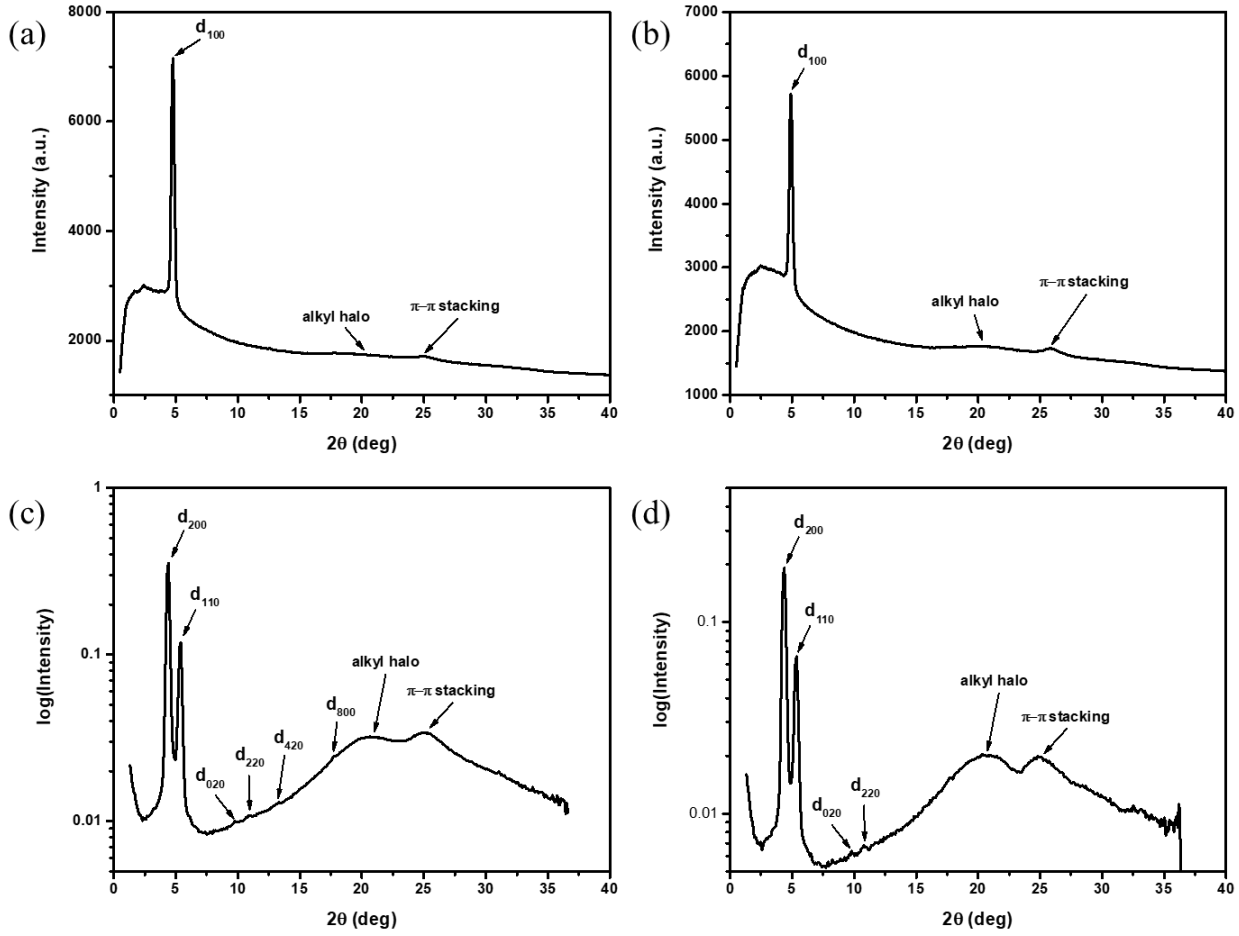


Figure S48. X-ray diffractograms of **dDBP(6)** at (a) 171 °C and (b) room temperature on the Rigaku instrument, and (c) 2 years and (d) 5 years at room temperature on the SAXS instrument.

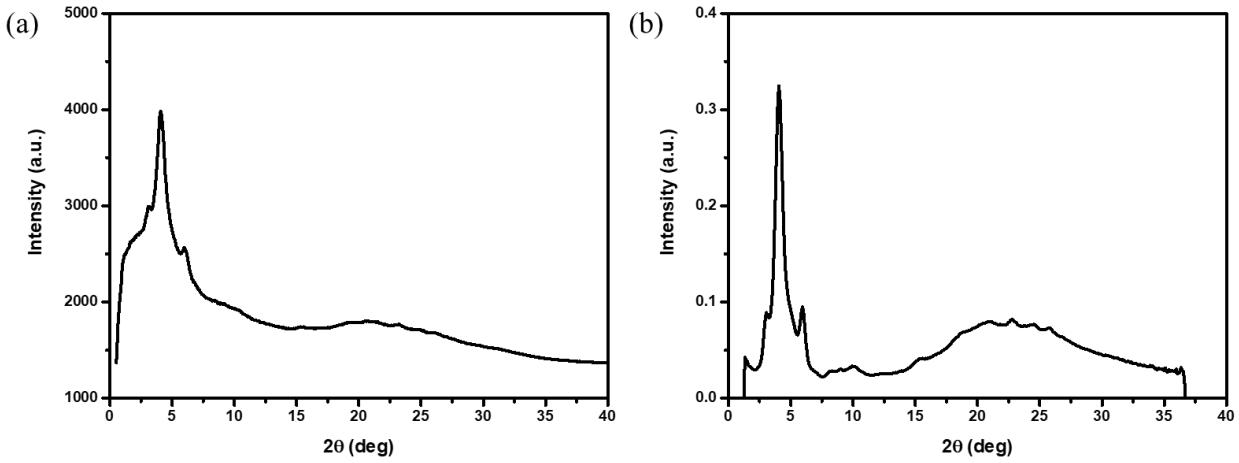


Figure S49. X-ray diffractograms of **dDBP(12)** at room temperature on (a) the Rigaku instrument and (b) the SAXS instrument.

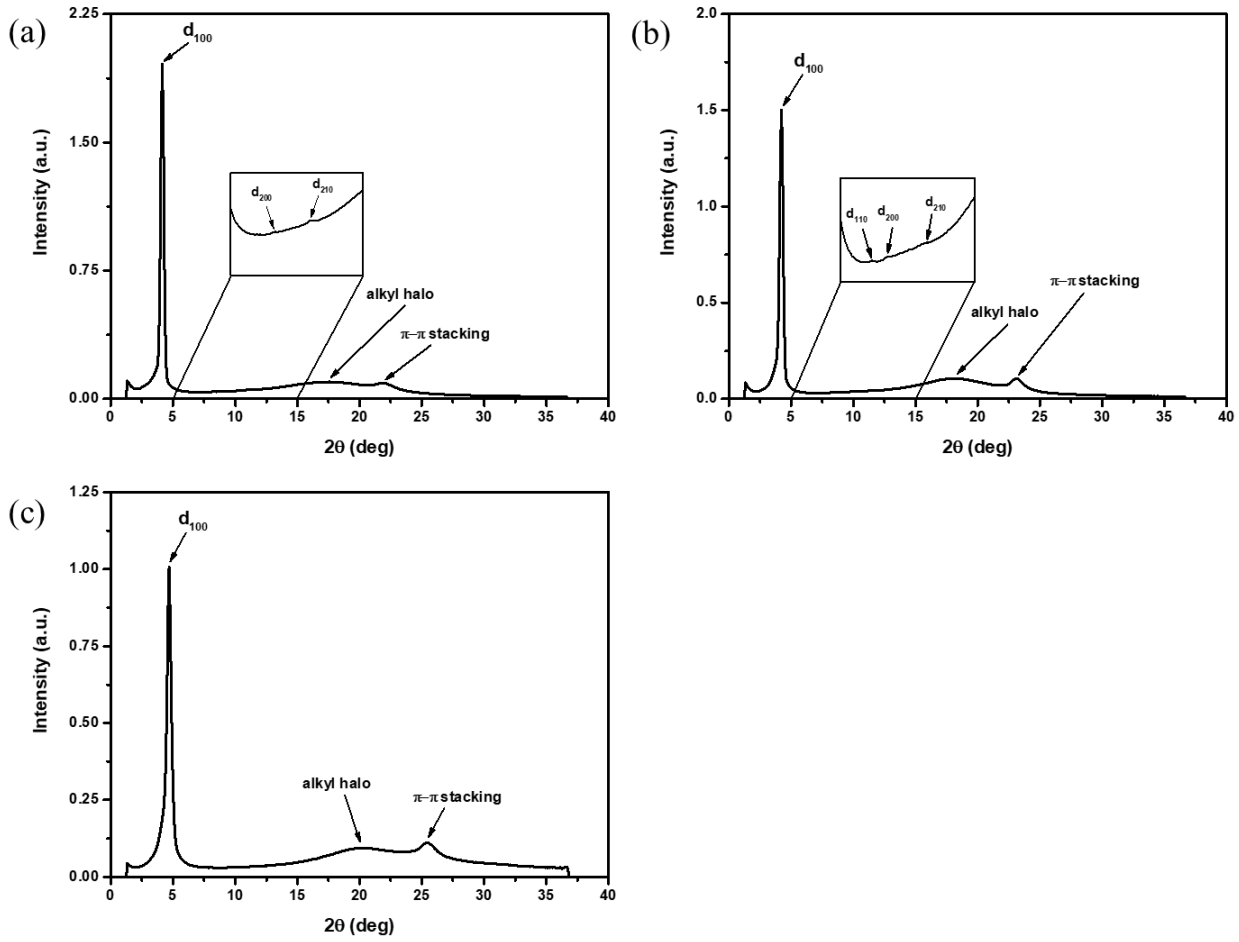


Figure S50. X-ray diffractograms of **dDBP(hyd,6)** at (a) 270 °C, (b) room temperature, and (c) 10 months at room temperature. All measurements were performed on the SAXS instrument.

Table S2. X-ray diffraction data of the three dodecyloxy DBP precursors.

Compound	T (°C)	d-spacings (Å)	Miller Index (hkl)	Phase (lattice constant)	LC Glass Stability
DBP(Me,12)	104	19.9	(100)	Col_h	N/A
		4.5	alkyl halo	(a = 23.0 Å)	
		3.5	π-π stacking		
DBP(Dod,12)	95	21.6	(100)	Col_h	N/A
		4.5	alkyl halo	(a = 25.0 A)	
		3.5	π-π stacking		
DBP(CA,12)	25		Crystalline solid		N/A

Table S3. X-ray diffraction data of the **DBP(PrOH,X)** derivatives.

Compound	T (°C)	d-spacings (Å)	Miller Index (hkl)	Phase (lattice constant)	LC Glass Stability
DBP(PrOH,1)	178	18.2	(100)	Col_h	N/A
		4.3	alkyl halo	(a = 21.0 Å)	
		3.5	π-π stacking		
DBP(PrOH,6)	188	19.1	(100)	Col_h	N/A
		4.5	alkyl halo	(a = 22.0 Å)	
		3.5	π-π stacking		
DBP(PrOH,12)	106	20.1	(100)	Col_h	N/A
		4.5	alkyl halo	(a = 23.2 Å)	
		3.4	π-π stacking		

Table S4. X-ray diffraction data of the **dDBP(X)** derivatives and **dDBP(hyd,6)**.

Compound	T (°C)	d-spacings d_{obs} / d_{calc} (Å)	Miller Index (hkl)	Phase (lattice constant)	LC Glass Stability
dDBP(1)	193	17.5	(100)	Col_h	>5 years
		4.7	alkyl halo	(a = 20.2 Å)	by DSC, POM, and XRD
		3.6	π-π stacking		
dDBP(6)	165	18.5	(100)	Col_h	>5 years
		4.5	alkyl halo	(a = 21.4 Å)	by DSC, POM, and XRD
		3.5	π-π stacking		
	25 (after ~1 year)	20.0 / 20.0	(200)	Col_r	
		16.5 / 16.5	(110)	(a = 40.0 Å)	
		9.0 / 9.0	(020)	(b = 18.1 Å)	
		8.1 / 8.2	(220)		
		6.7 / 6.7	(420)		
		4.9 / 5.0	(800)		
		4.3	alkyl halo		
		3.5	π-π stacking		
dDBP(12)	25	Crystalline solid			N/A
dDBP(hyd,6)	270	21.3 / 21.3	(100)	Col_h	N/A
		10.7 / 10.7	(200)	(a = 24.6 Å)	
		8.0 / 8.1	(210)		
		5.0	alkyl halo		
		4.0	π-π stacking		

6. Conformational Dynamics Data

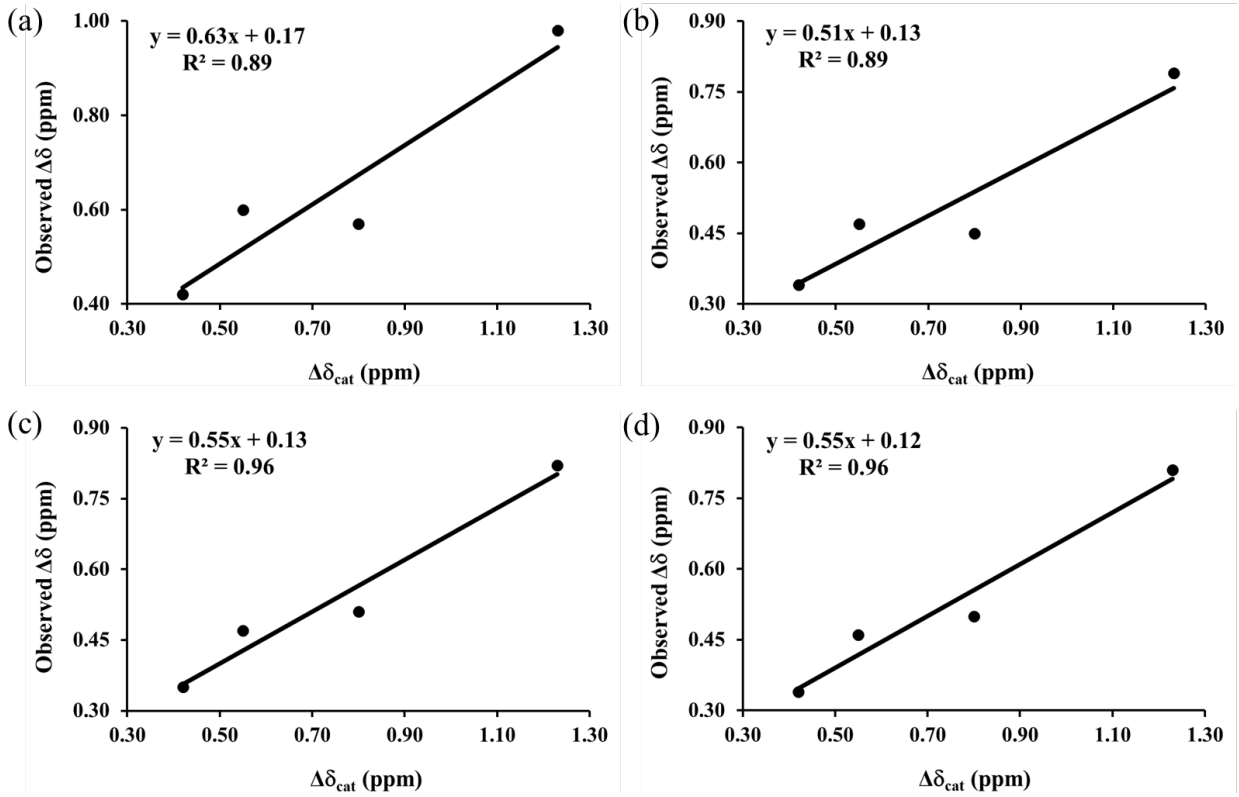


Figure S51. Plots of observed Δδ values against $\Delta\delta_{cat}$ for (a) **dDBP(H)**, (b) **dDBP(1)**, (c) **dDBP(6)**, and (d) **dDBP(12)**.

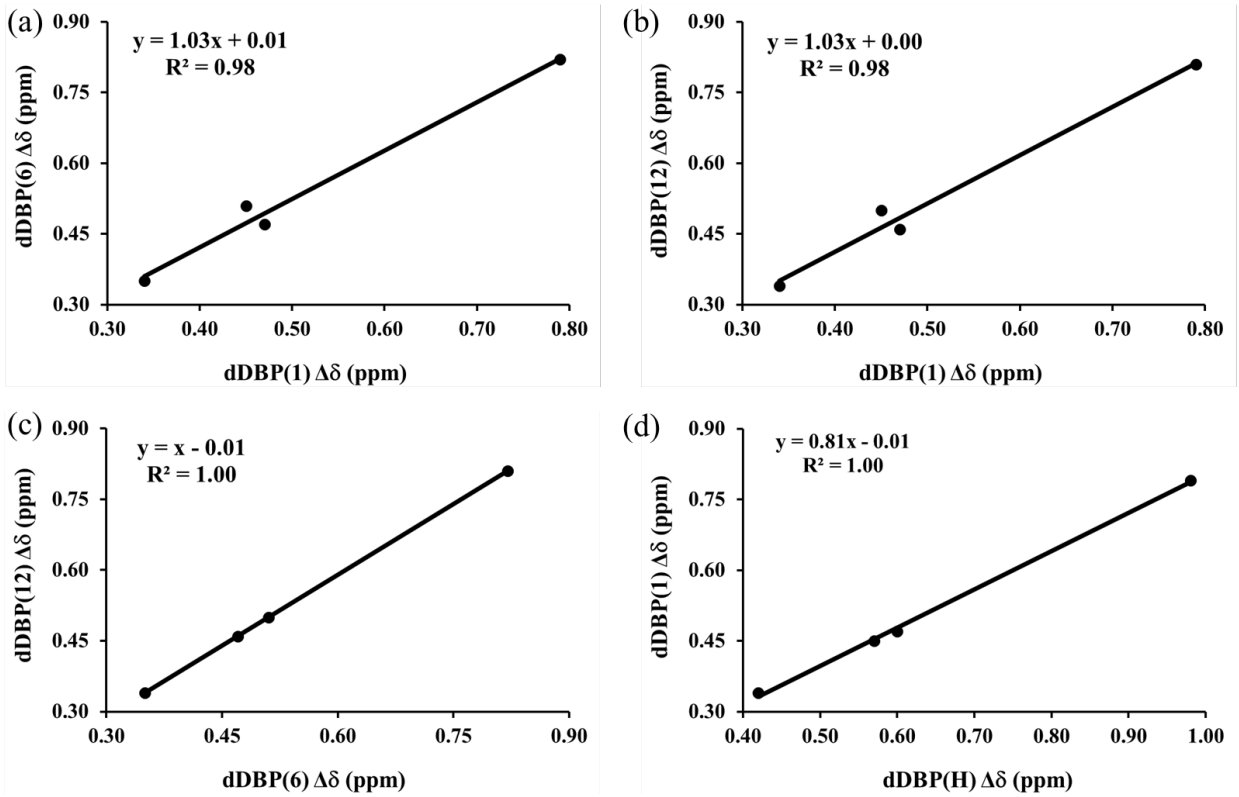


Figure S52. Plots of observed Δδ values for (a) **dDBP(6)** *versus* **dDBP(1)**, (b) **dDBP(12)** *versus* **dDBP(1)**, (c) **dDBP(12)** *versus* **dDBP(6)**, and (d) **dDBP(1)** *versus* **dDBP(H)**.

7. Modelling Schematics

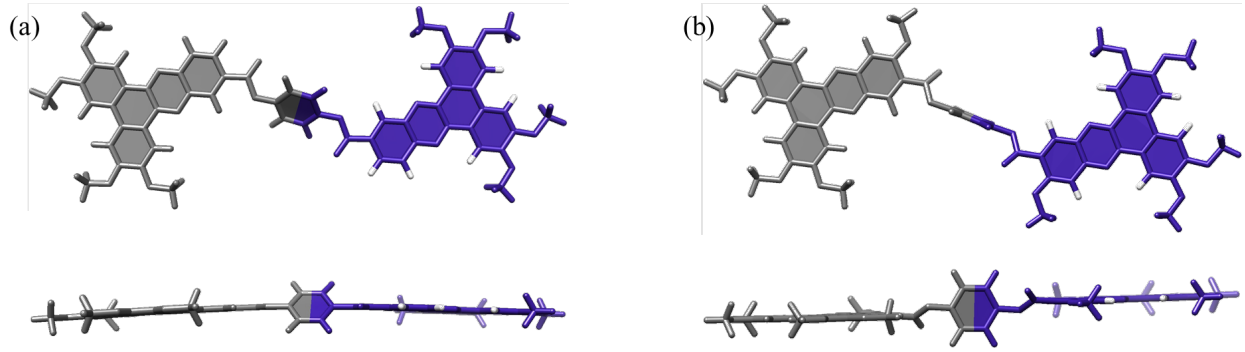


Figure S53. Models of dimers (a) **dDBP(hyd,H)** and (b) **dDBP(hyd,6)**, showing the top-down (top) and side (bottom) views.

8. Modelling Details

I. Optimization Methods

General Calculation Details

Preliminary calculations were carried out using Gaussian 09[2] in the gas phase. Calculations with a solvent (self-consistent reaction field (SCRF) method with chloroform) were attempted but no significant differences in the optimized geometries were observed. Unconstrained geometry optimizations for all compounds discussed in the manuscript were performed in multiple steps. First, a truncated dibenzo[a,c]phenazine (DBP) moiety with four peripheral methoxy chains in place of hexyloxy chains was constructed and optimized by density functional theory (DFT)[3] calculations using the Becke three parameter Lee-Yang-Parr (B3LYP) method[4,5] at the 6-31G(d) level[6,7] with the Grimme D3 dispersion correction (B3LYP-D3).[8] Calculations with a second polarization (6-31G(d,p)) were attempted on a number of conformers, but no differences were observed in the geometries.

Each ester, whether monomer or dimer, was constructed from this optimized DBP moiety as a starting point. For each DBP ester, multiple conformations are possible; the number of conformations for a given compound depends on the complexity and flexibility of the molecule (see Monomers and Dimers sections below). Once each conformation was constructed, unconstrained geometry optimizations were performed using Grimme's r2SCAN-3c method[9] in ORCA (version 5.0.3).[10]

Monomers

The two monoesters were constructed by taking the optimized DBP moiety, described above, and configured with the appropriate ester group to match the chemical structure of the monoester. For a given monomer, multiple conformations are possible, namely through the configuration of the ester group. The DBP methyl ester **DBP(Me,H)** (Figure S54) for example, shows the two distinct configurations the ester group can adopt: the carbonyl can be syn (Figure S54(b)) or anti (Figure S54(c)) to H_a on the DBP core. The two conformations of **DBP(Me,H)** are then optimized by DFT calculations in ORCA using r2SCAN-3c. The conformations of all monomers are summarized in the Results section (section III).

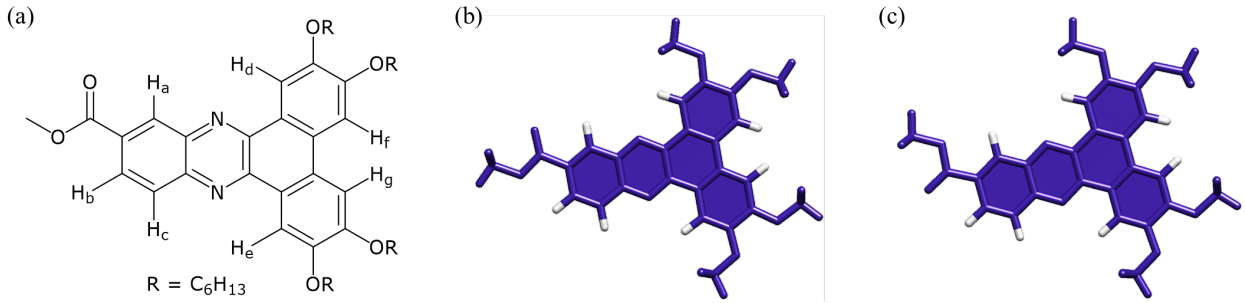


Figure S54. (a) Schematic of **DBP(Me,H)**, outlining the seven protons on the DBP ring. Note protons *d* and *e* cannot be distinguished by 2D NMR, and likewise for protons *f* and *g*. Assignment of protons *d* and *e* was determined by comparing the calculated chemical shifts to the experimental chemical shifts, and likewise for protons *f* and *g*. The two optimized conformers of **DBP(Me,H)** are shown on the right, where the carbonyl of the ester is either (b) syn or (c) anti to H_a. Hydrogens on the DBP core are shown in light grey.

Dimers

For the diesters, there are numerous conformations that can be adopted, including both folded and unfolded geometries. The number of conformers for a given dimer was determined by considering two geometrical factors: (i) the configuration of the two esters with respect to the linker and (ii) the conformations of the two esters in relation to the DBP core. These three factors determined the total number of conformations for a given dimer.

Figure S55 outlines all the possible conformations of the 1,3-propyl DBP diester (**dDBP(H)**). For **dDBP(H)**, there are (i) two possible configurations of the propyl linker: folded (**F**), where the dihedral angles between the carbons on the propyl linker are ~60° (gauche) and unfolded (**U**), where the dihedral angles between the carbons on the propyl linker are ~180° (anti). There are (ii) three possible configurations between the two esters and the linker: both carbonyls of the ester are syn to the methylene hydrogens (**+1**), one carbonyl is syn and one is anti to the methylene hydrogens (**0**), or both carbonyls are anti to the methylene hydrogens (**-1**) of the propyl group. Finally, there are (ii) three conformations between the two esters and the DBP core: both carbonyls of the ester are syn to H_a (**+1**), one carbonyl is syn and one is anti to H_a (**0**), or both carbonyls are anti to H_a (**-1**) of the DBP core.

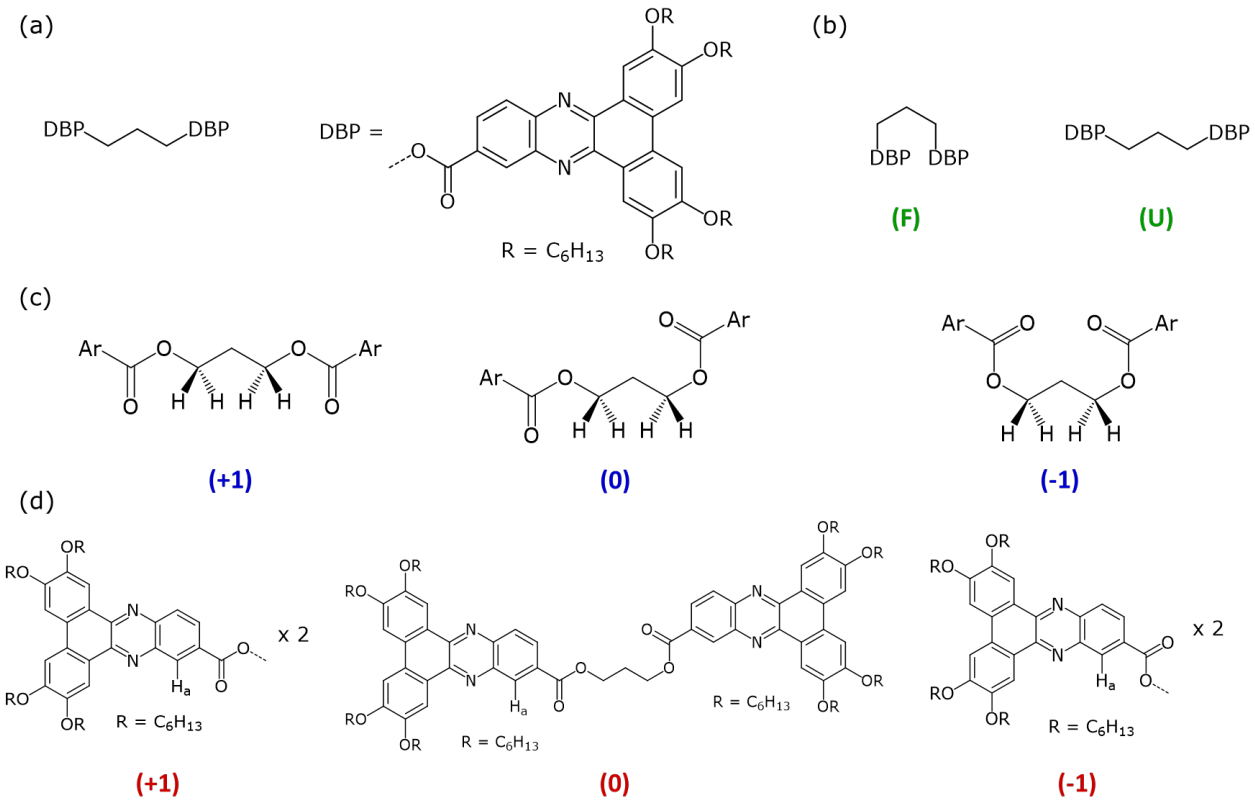


Figure S55. Schematics of (a) the chemical structure of **dDBP(H)**, (b) the folded (**F**) and unfolded (**U**) configurations of the propyl linker, (c) the three possible conformations of the diester with respect to the linker (Ar = DBP core), and (d) the three conformations between the diester and the DBP cores.

As outlined in Figure S55, each type of conformation is labelled to help keep track of all the possible conformations. For **dDBP(H)**, summing all configurations yields a total of 2·3·3 = 18 conformations; however, there are 20 conceivable conformations for **dDBP(H)** using the method of analysis outlined in Figure S55. The addition two conformations arise when (ii) is 0 and (iii) is 0; in this case, there are two possible scenarios: the carbonyl that is syn to the methylene hydrogens of the propyl linker can either be syn to H_a or anti to H_a of the DBP core, and *vice versa*. This scenario arises for both the folded and unfolded configuration, and therefore there are a total of 20 possible conformations for **dDBP(H)**. The other propyl dimer, **dDBP(1)**, was studied in a similar fashion.

Once the total number of conformers are determined for a dimer, each conformation was constructed by joining two DBP moieties, optimized according to the "General Calculation Details" section, with the appropriate linking group. Due to the size and flexibility of these molecules, it is often difficult to construct a good starting geometry that is close to the lowest energy structure for a given conformation. Performing an optimization from a reasonable starting geometry is vital because it can significantly reduce the cost of each calculation and increase the probability of reaching a local energetic minimum. To obtain a good starting geometry, conformations were first optimized with molecular mechanics using the universal force field (UFF).[11] The structures were then optimized again with DFT[3] calculations using the r2SCAN-3c method[9] in ORCA (version 5.0.3).[10]

To validate the reliability of pre-optimizing the conformations with molecular mechanics, independent calculations on a few conformations with and without a molecular mechanics pre-optimization were performed. Results showed that both methods converged to the same local conformational minimum (*i.e.,* the same optimized structure was obtained), thereby validating the use of a pre-optimization. As expected, the calculations without the molecular mechanics pre-optimization were more computationally expensive.

II. NMR Calculations

General Calculation Details

The ^{1}H-NMR of each folded conformation was calculated from the optimized geometries. The standard Gauge-Independent Atomic Orbital (GIAO) approach[12] was used for the ^{1}H-NMR calculations at the DFT level (B3LYP-D3, 6-31G(d)). The GIAO approach has proven useful in calculating the magnetic shielding of protons for a wide variety of molecules.[13,14] The calculated ^{1}H-NMRs for each conformation was then compared with the experimental ^{1}H-NMR data. The details of these analyses are summarized in the "Monomers" and "Dimers" sections below.

Monomers

For each monoester, the ^{1}H-NMR of the optimized conformations was calculated according to the GIAO method described above. For each conformer of a given monomer, the chemical shifts of the seven aromatic protons on the DBP moiety were recorded after being referenced to TMS (B3LYP/6-311+G(2d,p) GIAO) in Gaussian 09.[2] The chemical shift of each aromatic proton for a given monoester will be denoted as the δ_m. Each monoester has multiple possible conformations as described previously. The conformers do not vary appreciably in energy – most conformers are within 5 kcal/mol of each other; hence, the calculated δ_m for each monoester was determined by taking a non-weighted average of the chemical shift values amongst all the possible conformers. To verify the accuracy of the ^{1}H-NMR calculations, the average calculated δ_m values were compared with the experimental δ_m values (Figure S56). All monoesters displayed a fit of $R^2 \geq 0.96$; hence, the NMR calculations do appear to accurately depict the experimental aromatic region of the ^{1}H-NMR.

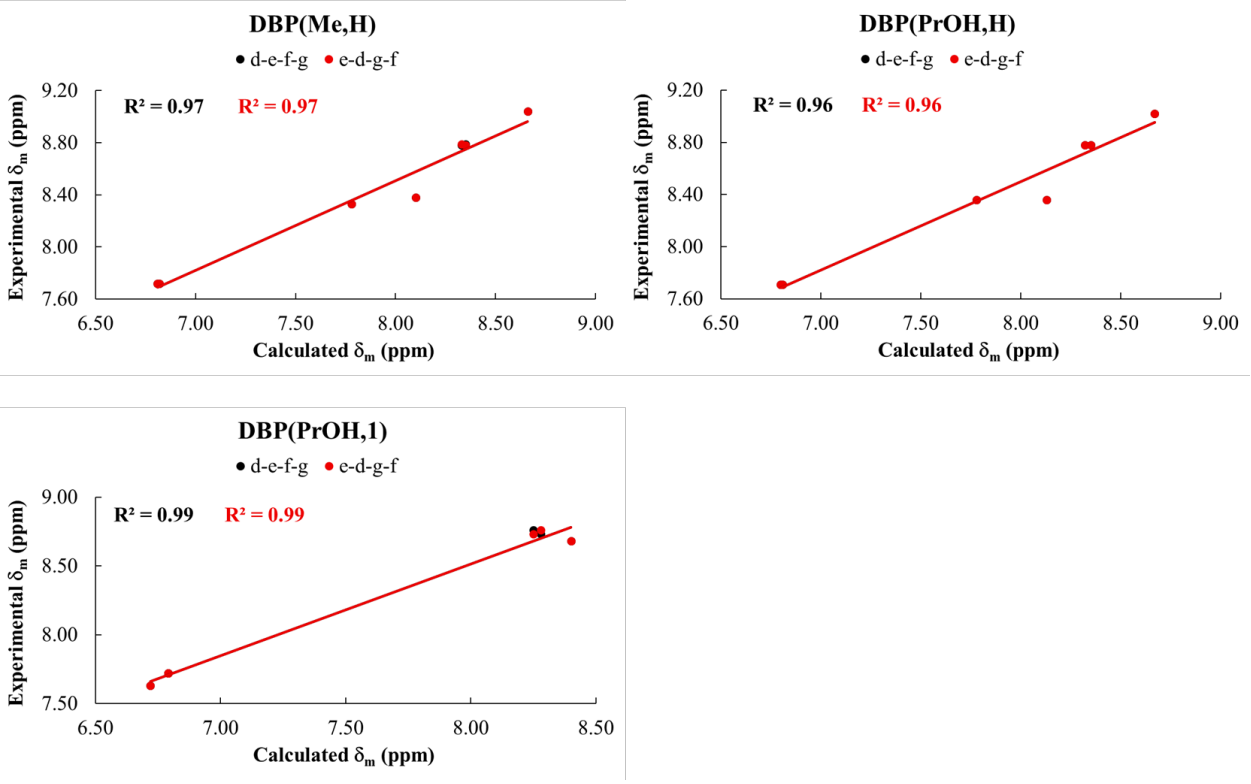


Figure S56. Experimental δ_m *versus* calculated δ_m plots for **DBP(Me,H)**, **DBP(PrOH,H)**, and **DBP(PrOH,1)**. For each graph, two series are plotted: d-e-f-g and e-d-g-f. These two series are plotted separately because, as elucidated in Figure S54, proton pairs *d*/*e* and *f*/*g* are indistinguishable by experimental NMR methods; however, HSQC and HMBC NMR experiments do show proton pairs *d*/*f* and *e*/*g* are on the same ring. Two possibilities therefore arise: series d-e-f-g (black), which assumes protons *d* and *f* are downfield relative to protons *e* and *g*, respectively, and series e-d-g-f (red), which assumes protons *e* and *g* are downfield relative to protons *d* and *f*, respectively.

Dimers

NMR calculations were performed on all optimized folded conformations for **dDBP(H)** and **dDBP(1)**. For each conformer, the chemical shifts of the aromatic protons on the DBP moiety were recorded after being referenced to TMS (B3LYP/6-311+G(2d,p) GIAO) in Gaussian 09.[2] The degree of upfield shift, Δδ, for each aromatic proton in a folded conformer with respect to its monomer (**DBP(Me,H)** and **DBP(PrOH,1)**) was calculated according to equation (S1):

$$\Delta\delta = \delta_m - \delta_d \quad \text{(S1)}$$

where δ_m and δ_d are the chemical shifts of each aromatic proton for a monomer and dimer, respectively. For each dimer, the observed Δδ values were plotted against the calculated Δδ values for each folded conformation to determine which conformer best represents the upfield shift in solution. These plots are shown in the Results section, along with the NMR fit (R^2 value) and slope of the line.

III. Results

Monomers

This section describes the total number of conformations, the relative energy of each conformation, ΔE, and the geometry of each conformation for each monoester, all summarized in Table S5-S8 and Figure S57Figure S59. The ΔE for each conformation is proportionate to the lowest energy conformer; the lowest energy conformer for each monoester is set to 0 kcal/mol.

DBP(MeE)

Two conformations were analyzed for **DBP(Me,H)**, as described in Figure S54.

Table S5. The total number of conformations, energies, relative energies, and number of imaginary frequencies for each conformer of **DBP(Me,H)**.

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	(+1/2)	-1564.5821	+0.3	0
2	(-1/2)	-1564.5827	0.0	0

DBP(1)

This previously reported monomer[15] was analyzed to determine the preferred orientation of the methoxy group. Five conformations were analyzed, which arise from the following geometrical factors: there are five configurations between the methoxy group and the DBP core – dihedral angles of 0°, 45°, 90°, 135°, or 180° relative to H(a) (see Figure S54 for schematic of the DBP core).

Table S6. The total number of conformations, energies, relative energies, and number of imaginary frequencies for each conformer of **DBP(1)**.

Number	Input Dihedral Angle (deg)	Output Diehdral Angle (deg)	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	0	0	-1451.2378	0.0	0
2	45	0	-1451.2378	0.0	0
3	90	180	-1451.2346	+2.0	0
4	135	180	-1451.2345	+2.1	0
5	180	180	-1451.2346	+2.1	0

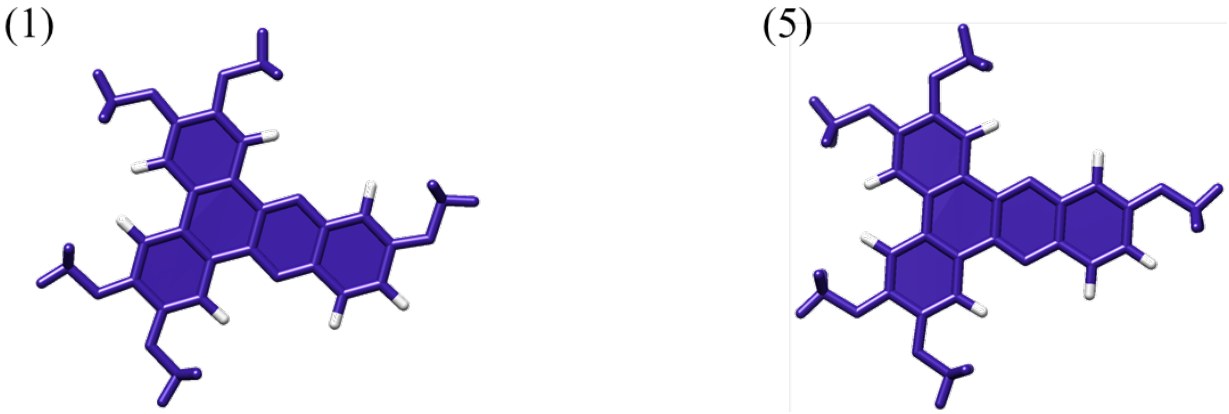


Figure S57. Schematics of the 2 optimized conformations for **DBP(1)**. The number displayed in the figure corresponds to the conformation number in Table S6. Hydrogens on the DBP core are shown in light grey.

DBP(PrOH,H)

Four conformations were analyzed for **DBP(PrOH,H)**, which arise from the following geometrical factors: there are two possible configurations between the ester and the propyl chain – the carbonyl is syn (**+1/2**) or anti (**-1/2**) to the methylene hydrogens on the adjacent carbon of the 3-hydroxypropyl group. There are two starting configurations between the ester and the DBP core – the carbonyl is syn (**+1/2**) or anti (**-1/2**) to H(a) of the DBP core (see Figure S54 for schematic of the DBP core).

Table S7. The total number of conformations, energies, relative energies, and number of imaginary frequencies for each conformer of **DBP(PrOH,H)**.

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	(**+1/2**, **+1/2**)	-1718.3964	+0.3	0
2	(**-1/2**, **-1/2**)	-1718.3969	0.0	1
3	(**-1/2**, **+1/2**)	-1718.3962	+0.4	0
4	(**-1/2**, **-1/2**)	-1718.3966	+0.2	0

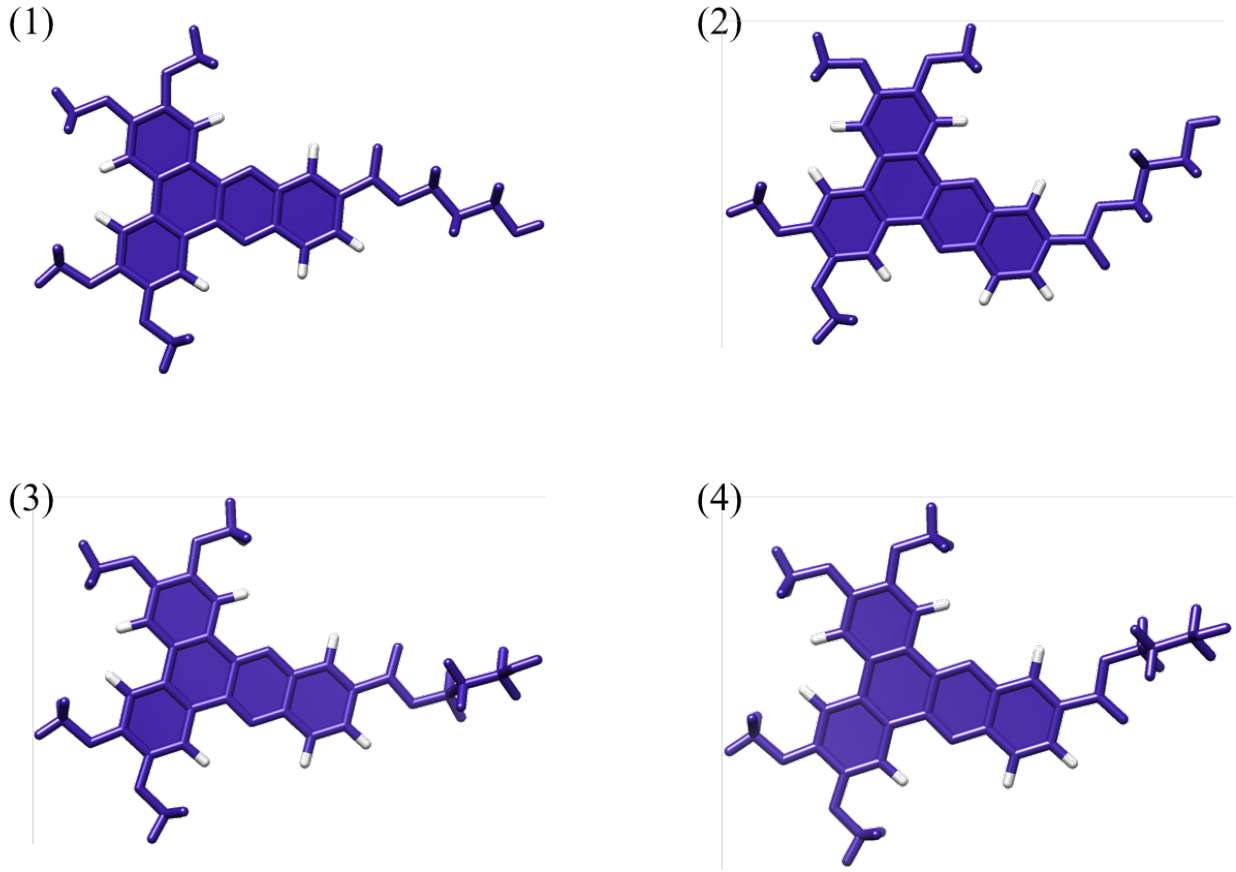


Figure S58. Schematics of all 4 conformations for **DBP(PrOH,H)**. The number displayed in the figure corresponds to the conformation number in Table S7. Hydrogens on the DBP core are shown in light grey.

DBP(PrOH,1)

Four conformations were analyzed for **DBP(PrOH,1)**, which arise from the following geometrical factors: there are two possible configurations between the ester and the propyl chain – the carbonyl is syn (**+1/2**) or anti (**-1/2**) to the methylene hydrogens on the adjacent carbon of the 3-hydroxypropyl group. There are two starting configurations between the ester and the DBP core – the carbonyl is syn (**+1/2**) or anti (**-1/2**) to H(a) of the DBP core (see Figure S54 for schematic of the DBP core). For all 4 conformers, the *ortho* methoxy group is initially set planar to the DBP core, with the methyl group pointing away from the ester (steric bulk prevents the methoxy group from pointing towards the ester). This configuration was found to be energetically favourable according to calculations of **DBP(1)** described above.

Table S8. The total number of conformations, energies, relative energies, and number of imaginary frequencies for each conformer of **DBP(PrOH,1)**.

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	(+1/2, +1/2)	-1832.8965	0.0	1
2	(-1/2, -1/2)	-1832.8963	+0.1	1
3	(-1/2, +1/2)	-1832.8961	+0.2	1
4	(-1/2, -1/2)	-1832.8962	+0.2	0

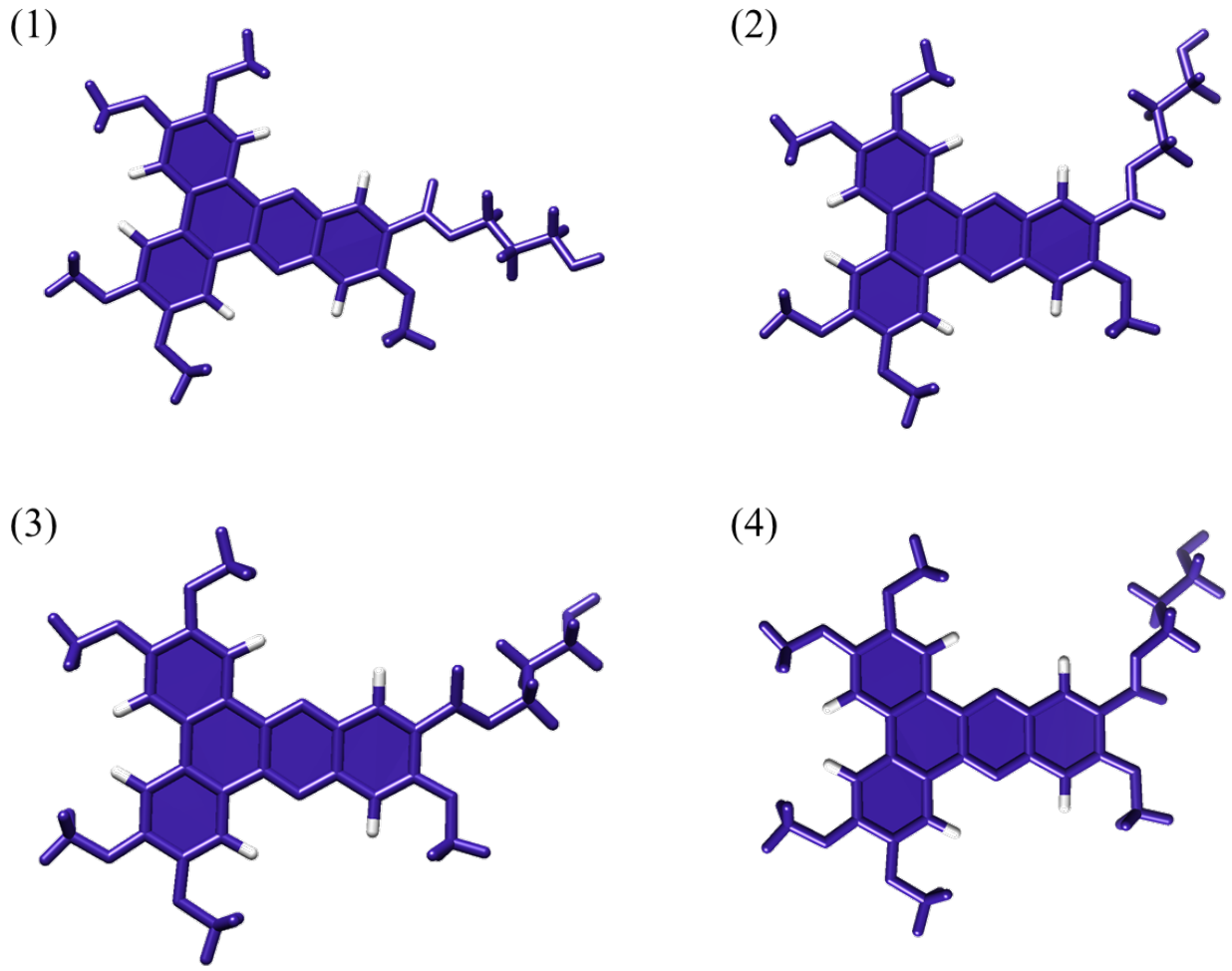


Figure S59. Schematics of all 4 conformations for **DBP(PrOH,1)**. The number displayed in the figure corresponds to the conformation number in Table S8. Hydrogens on the DBP core are shown in light grey.

Dimers

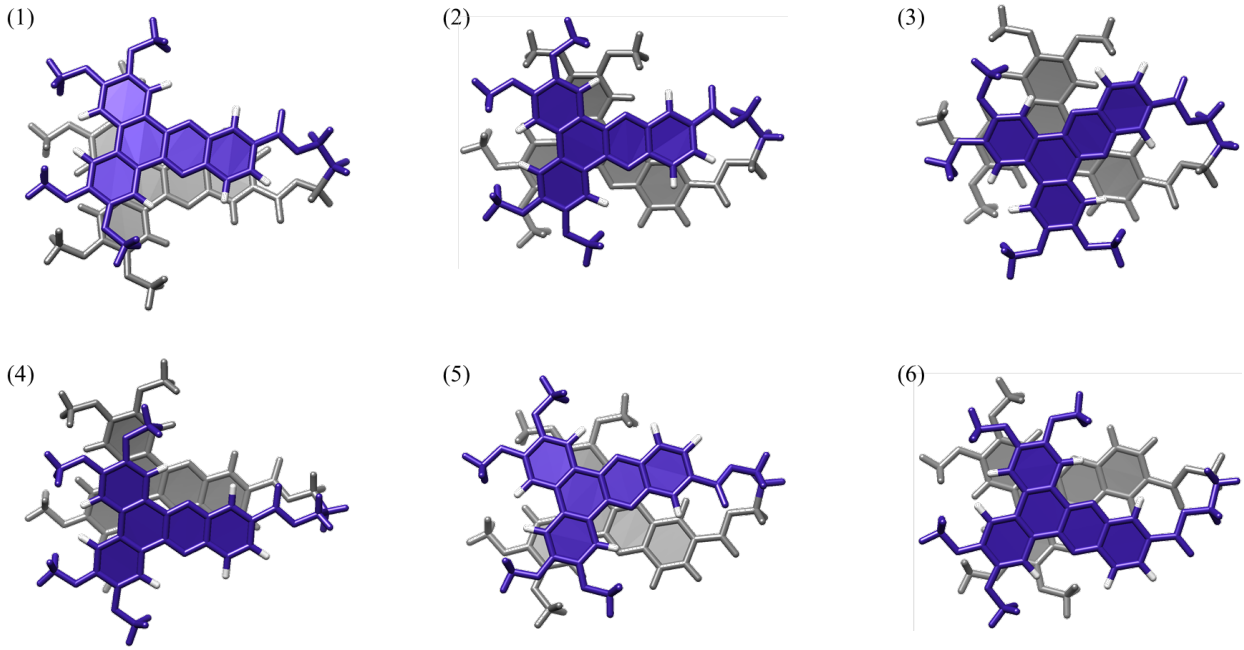
This section describes the total number of conformations, the relative energy of each conformation, ΔE, the geometry of each conformation, and the observed Δδ *versus* calculated Δδ ^{1}H NMR fits for each folded conformation of **dDBP(H)** and **dDBP(1)**. The ΔE for each conformation is proportionate to the lowest energy conformation; the lowest energy conformation for each dimer is set at 0 kcal/mol. For each experimental Δδ *versus* calculated Δδ ^{1}H NMR graph, two series are plotted: d-e-f-g and e-d-g-f. These two series are plotted separately because, as elucidated in Figure S56, proton pairs *d*/*e* and *f*/*g* are indistinguishable by experimental NMR methods; however, HSQC and HMBC NMR experiments do show protons *d*/*f* and *e*/*g* are on the same ring. Therefore, two possibilities arise: series d-e-f-g (black), which assumes protons *d* and *f* are downfield relative to protons *e* and *g*, respectively, and series e-d-g-f (blue), which assumes protons *e* and *g* are downfield relative to protons *d* and *f*, respectively.

dDBP(H)

Twenty conformations were analyzed for **dDBP(H)**, ten folded (**F**) and ten unfolded (**U**). The folded conformations are generated by adjusting the dihedral angles of the three carbons on the propyl linker to ~60° (gauche). The unfolded conformations are generated by adjusting the dihedral angles of the three carbons on the propyl linker to ~180° (anti). The 10 folded and 10 unfolded conformations arise from the following geometrical factors: there are three configurations between the two esters and the propyl linker – both carbonyls are syn (**+1**), one carbonyl is syn and the other is anti (**0**), or both carbonyls are anti (**-1**) to the methylene hydrogens on the adjacent carbons of the propyl chain. There are three configurations between the two esters and the DBP core – both carbonyls are syn (**+1**), one carbonyl is syn and the other is anti (**0**), or both carbonyls are anti (**-1**) to H(a) on the DBP core (see Figure S54 for schematic of the DBP core).

Table S9. The total number of conformations, energies, relative energies, number of imaginary frequencies, and R^2 fit and slope from the observed Δδ *versus* $\Delta\delta_{calc}$ plots for each conformer of **dDBP(H)**. *Carbonyl syn to the methylene Hs is anti to H(a); ** carbonyl anti to the methylene Hs is anti to H(a).

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq	NMR R^2 Fit
1	(F, +1, +1)	-3167.3123	+8.7	0	0.17
2	(F, +1, 0)	-3167.3159	+6.5	5	0.72
3	(F, +1, -1)	-3167.3133	+8.1	0	0.77
4	(F, 0, +1)	-3167.3187	+4.7	0	0.00
5	(F, 0, 0)*	-3167.3263	0.0	0	0.80
6	(F, 0, 0)**	-3167.3263	0.0	0	0.80
7	(F, 0, -1)	-3167.3200	+3.9	1	0.67
8	(F, -1, +1)	-3167.3215	+3.0	0	0.44
9	(F, -1, 0)	-3167.3202	+3.8	0	0.12
10	(F, -1, -1)	-3167.3219	+2.7	0	0.86
11	(U, +1, +1)	-3167.2814	+28.1	0	N/A
12	(U, +1, 0)	-3167.2819	+27.8	0	N/A
13	(U, +1, -1)	-3167.2830	+27.2	0	N/A
14	(U, 0, +1)	-3167.2816	+28.0	0	N/A
15	(U, 0, 0)*	-3167.2821	+27.7	0	N/A
16	(U, 0, 0)**	-3167.2821	+27.7	0	N/A
17	(U, 0, -1)	-3167.2824	+27.5	0	N/A
18	(U, -1, +1)	-3167.2818	+27.9	0	N/A
19	(U, -1, 0)	-3167.2822	+27.6	0	N/A
20	(U, -1, -1)	-3167.2828	+27.3	0	N/A



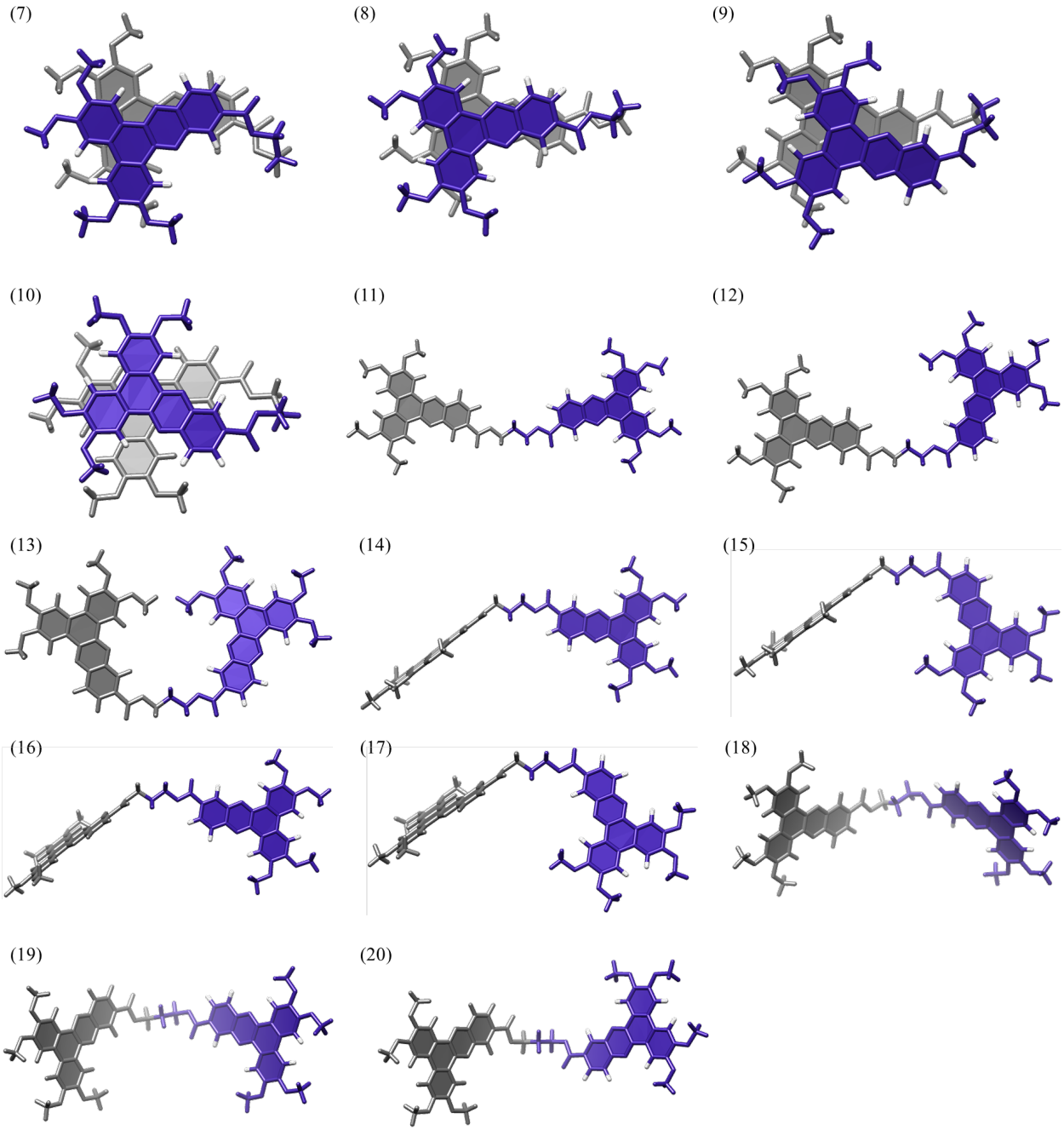
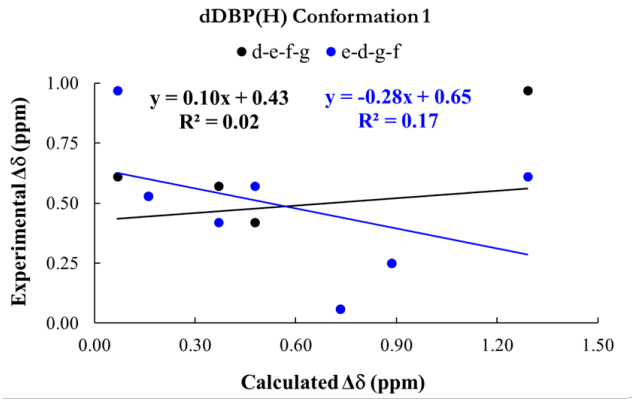
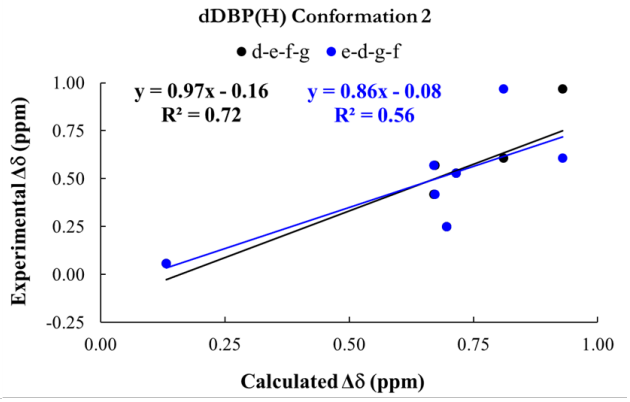
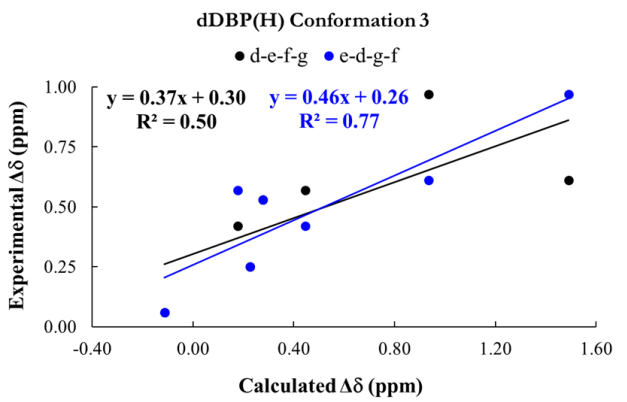
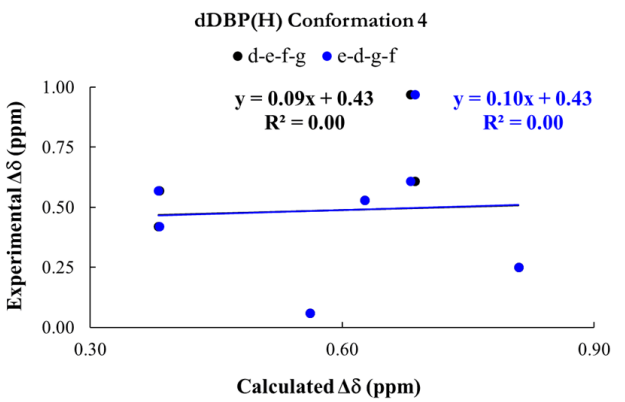


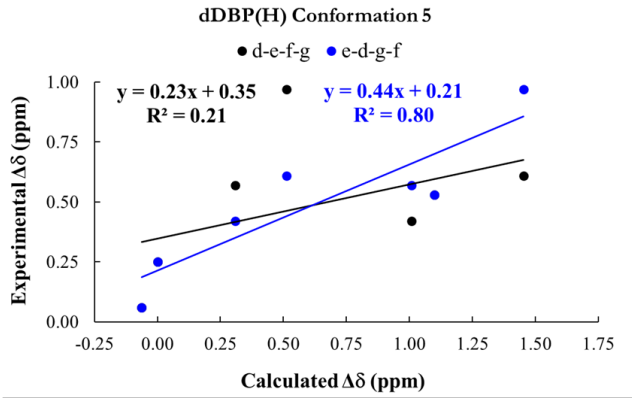
Figure S60. Schematics of all 20 conformations for **dDBP(H)**. The number displayed in the figure corresponds to the conformation number in Table S9. For each conformation, the DBP core that appears in front (or on the right for unfolded conformations) is coloured in violet, and the other DBP core is coloured in grey. Hydrogens on the DBP core in violet are shown in light grey.

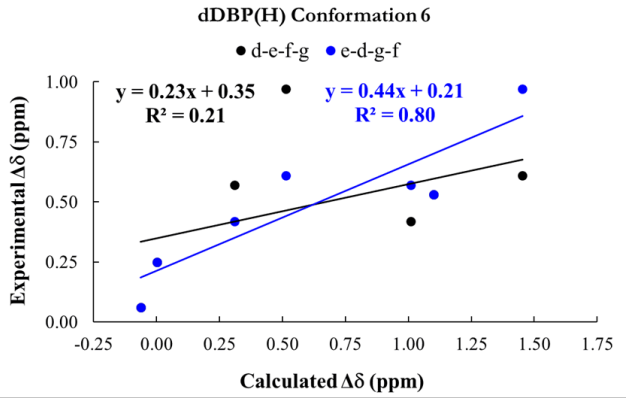

dDBP(H) Conformation 1
d-e-f-g
e-d-g-f
y = 0.10x + 0.43
R² = 0.02
y = -0.28x + 0.65
R² = 0.17
Experimental Δδ (ppm)
Calculated Δδ (ppm)

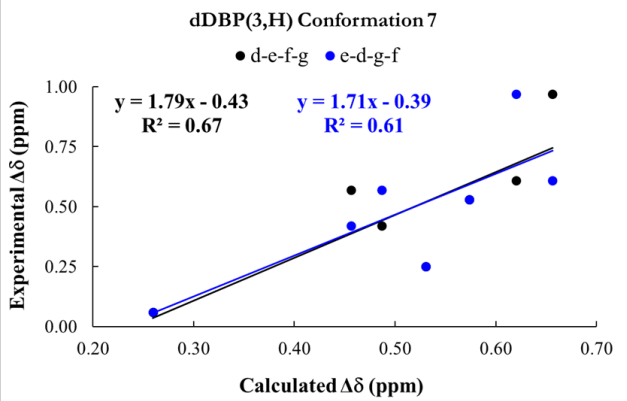

dDBP(H) Conformation 2
d-e-f-g
e-d-g-f
y = 0.97x - 0.16
R² = 0.72
y = 0.86x - 0.08
R² = 0.56
Experimental Δδ (ppm)
Calculated Δδ (ppm)

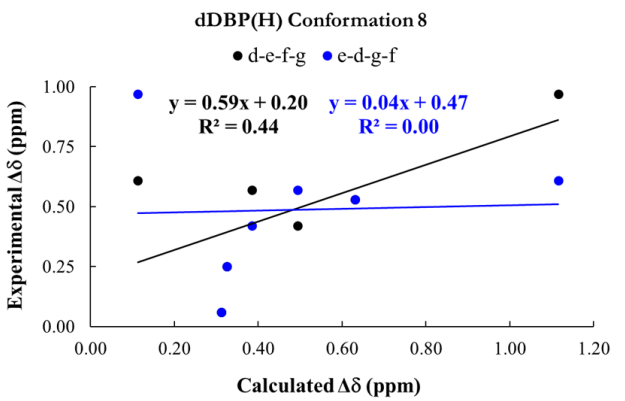

dDBP(H) Conformation 3
d-e-f-g
e-d-g-f
y = 0.37x + 0.30
R² = 0.50
y = 0.46x + 0.26
R² = 0.77
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(H) Conformation 4
d-e-f-g
e-d-g-f
y = 0.09x + 0.43
R² = 0.00
y = 0.10x + 0.43
R² = 0.00
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(H) Conformation 5
d-e-f-g
e-d-g-f
y = 0.23x + 0.35
R² = 0.21
y = 0.44x + 0.21
R² = 0.80
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(H) Conformation 6
d-e-f-g
e-d-g-f
y = 0.23x + 0.35
R² = 0.21
y = 0.44x + 0.21
R² = 0.80
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(3,H) Conformation 7
d-e-f-g
e-d-g-f
y = 1.79x - 0.43
R² = 0.67
y = 1.71x - 0.39
R² = 0.61
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(H) Conformation 8
d-e-f-g
e-d-g-f
y = 0.59x + 0.20
R² = 0.44
y = 0.04x + 0.47
R² = 0.00
Experimental Δδ (ppm)
Calculated Δδ (ppm)

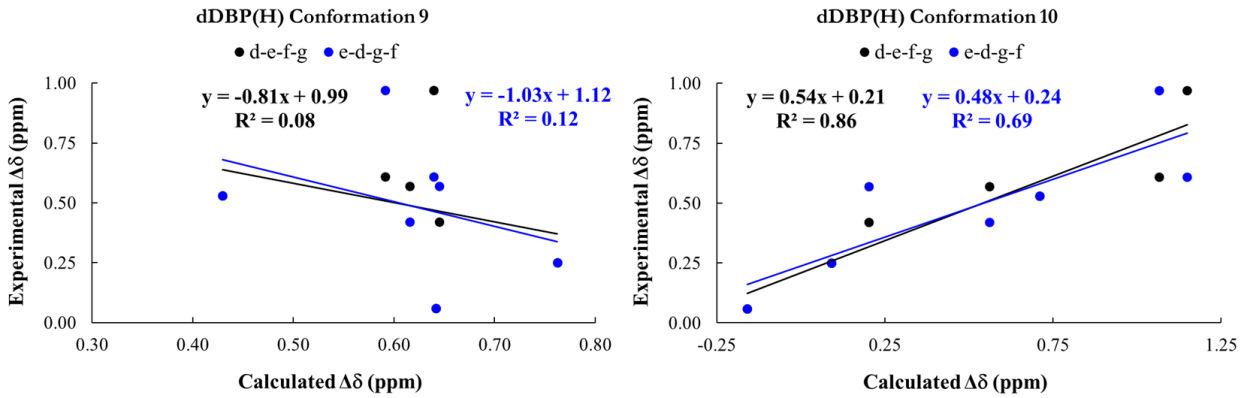


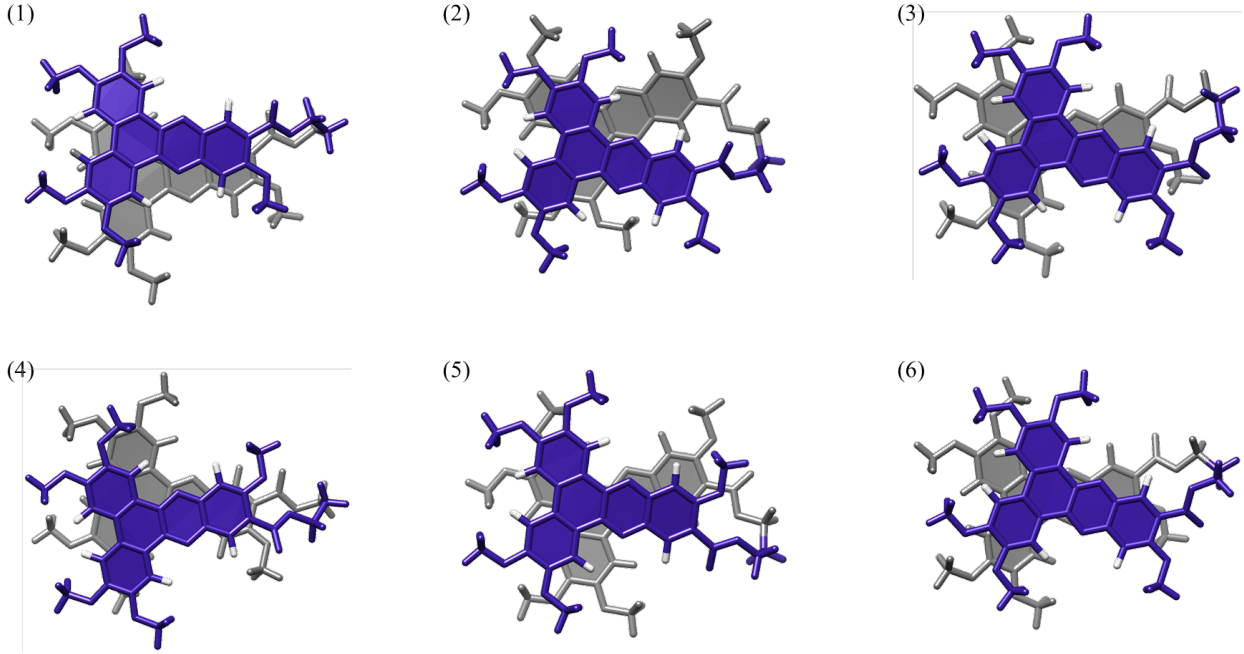
Figure S61. Experimental Δδ *versus* calculated Δδ NMR plots for each of the 10 folded conformations analyzed for **dDBP(H)**. The title of each plot refers to the conformation number in Table S9 and Figure S60.

dDBP(1)

Twenty conformations were analyzed for **dDBP(1)**, ten folded (**F**) and ten unfolded (**U**). The folded conformations are generated by adjusting the dihedral angles of the three carbons on the propyl linker to ~60° (gauche). The unfolded conformations are generated by adjusting the dihedral angles of the three carbons on the propyl linker to ~180° (anti). For all 20 conformers, the *ortho* methoxy group is initially set planar to the DBP core, with the methyl group pointing away from the ester (steric bulk prevents the methoxy group from pointing towards the ester). This configuration was found to be energetically favourable according to calculations of **DBP(1)**. The 10 folded and 10 unfolded conformations arise from the following geometrical factors: there are three configurations between the two esters and the propyl linker – both carbonyls are syn (**+1**), one carbonyl is syn and the other is anti (**0**), or both carbonyls are anti (**-1**) to the methylene hydrogens on the adjacent carbons of the propyl chain. There are three configurations between the two esters and the DBP core – both carbonyls are syn (**+1**), one carbonyl is syn and the other is anti (**0**), or both carbonyls are anti (**-1**) to H(a) on the DBP core (see Figure S54 for schematic of the DBP core).

Table S10. The total number of conformations, energies, relative energies, number of imaginary frequencies, and R^2 fit and slope from the observed Δδ *versus* $\Delta\delta_{calc}$ plots for each conformer of **dDBP(1)**. *Carbonyl syn to the methylene Hs is anti to H(a); **carbonyl anti to the methylene Hs is anti to H(a).

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq	NMR R^2 Fit
1	(F, +1, +1)	-3396.3216	+4.4	0	0.17
2	(F, +1, 0)	-3396.3258	+1.7	0	0.73
3	(F, +1, -1)	-3396.3263	+1.5	1	0.38
4	(F, 0, +1)	-3396.3250	+2.3	0	0.39
5	(F, 0, 0)*	-3396.3276	+0.6	0	0.17
6	(F, 0, 0)**	-3396.3286	0.0	0	0.23
7	(F, 0, -1)	-3396.3211	+4.7	0	0.69
8	(F, -1, +1)	-3396.3212	+4.6	0	0.60
9	(F, -1, 0)	-3396.3265	+1.4	0	0.67
10	(F, -1, -1)	-3396.3286	0.0	0	0.23
11	(U, +1, +1)	-3396.2817	+29.5	0	N/A
12	(U, +1, 0)	-3396.2816	+29.5	0	N/A
13	(U, +1, -1)	-3396.2817	+29.5	0	N/A
14	(U, 0, +1)	-3396.2817	+29.4	0	N/A
15	(U, 0, 0)*	-3396.2894	+24.6	0	N/A
16	(U, 0, 0)**	-3396.2816	+29.5	0	N/A
17	(U, 0, -1)	-3396.2814	+29.6	0	N/A
18	(U, -1, +1)	-3396.2806	+30.1	0	N/A
19	(U, -1, 0)	-3396.2812	+29.7	0	N/A
20	(U, -1, -1)	-3396.2803	+30.3	0	N/A



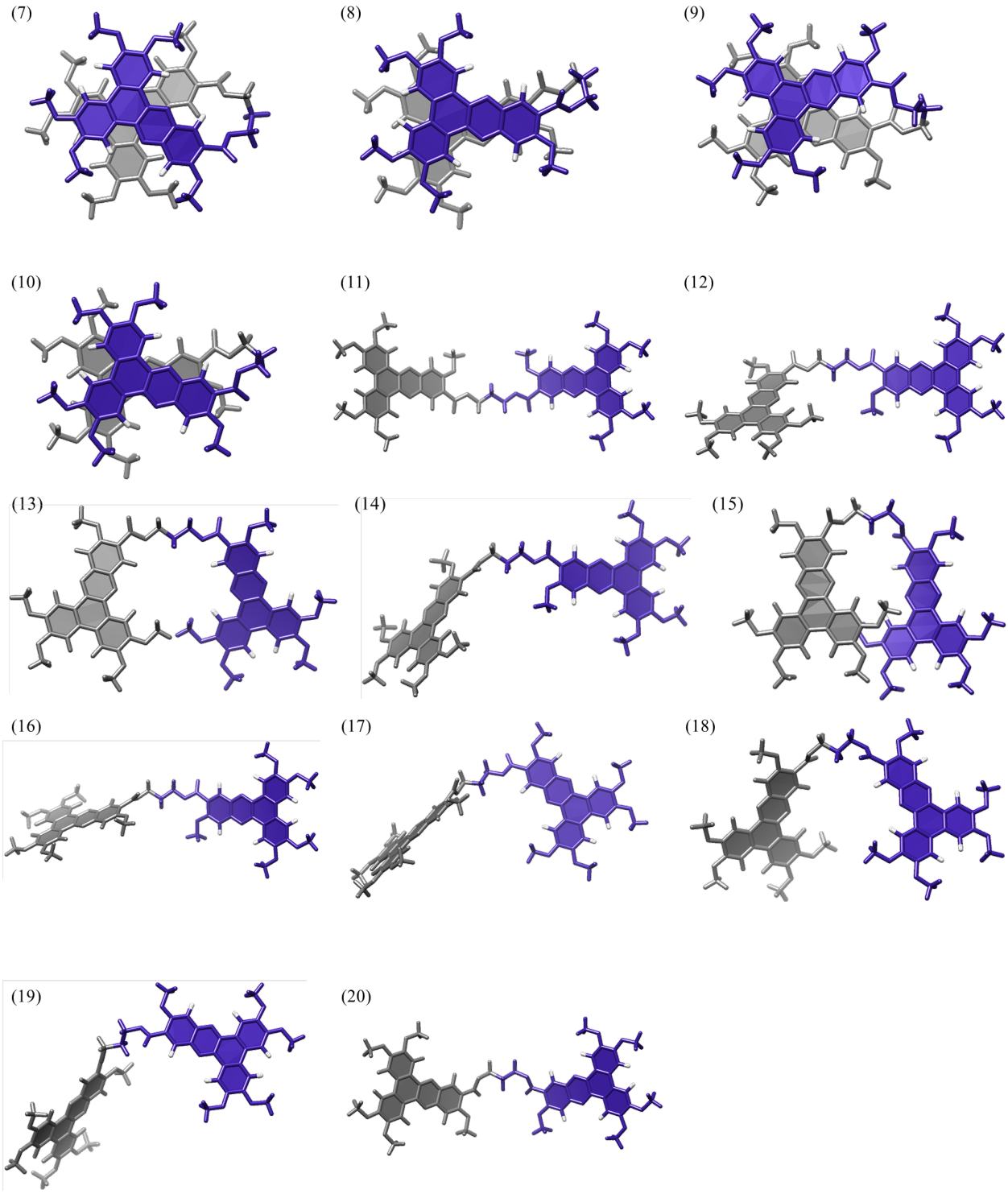
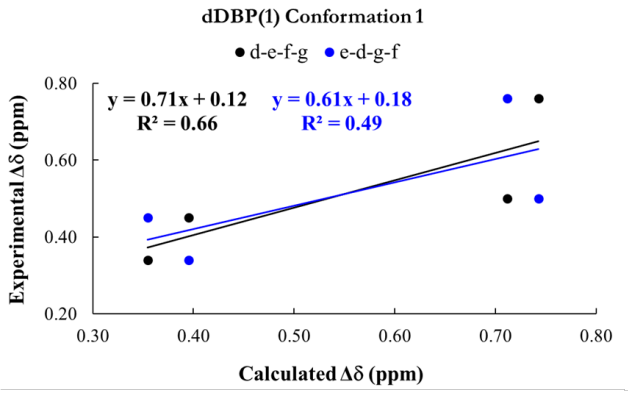
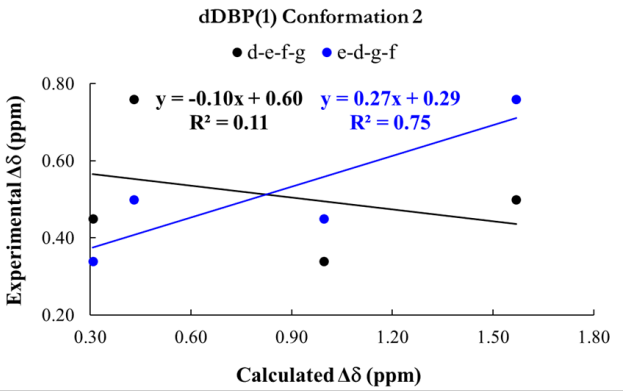
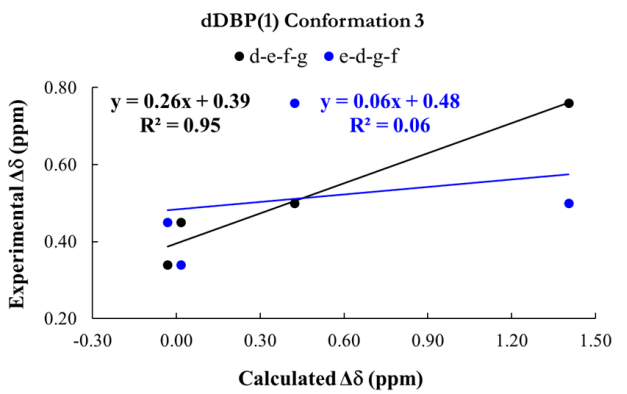
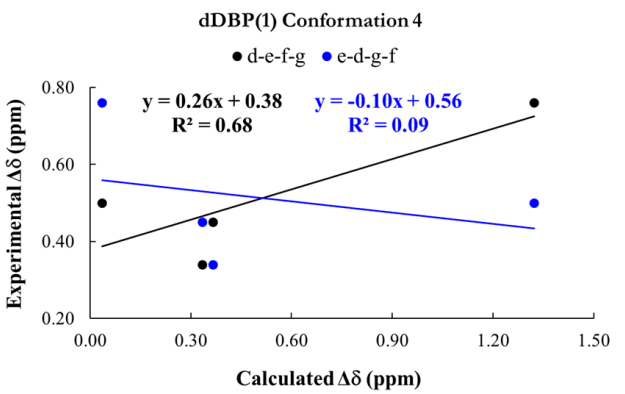


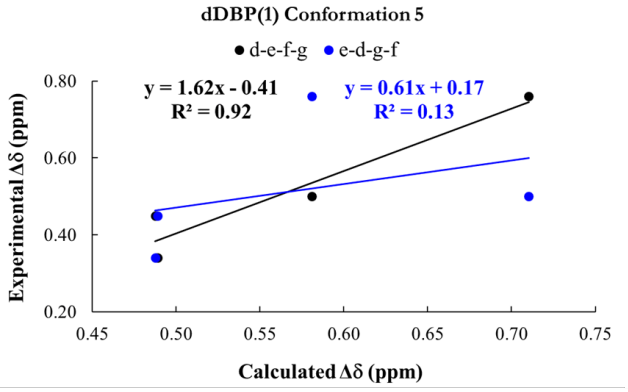
Figure S62. Schematics of all 20 conformations for **dDBP(1)**. The number displayed in the figure corresponds to the conformation number in Table S10. For each conformation, the DBP core that appears in front (or on the right for unfolded conformations) is coloured in violet, and the other DBP core is coloured in grey. Hydrogens on the DBP core in violet are shown in light grey.

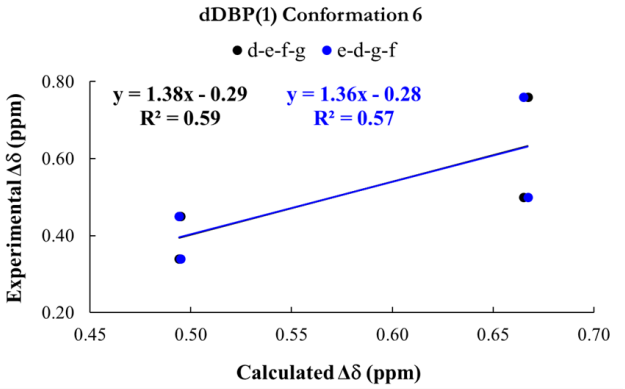

dDBP(1) Conformation 1
d-e-f-g
e-d-g-f
y = 0.71x + 0.12
R² = 0.66
y = 0.61x + 0.18
R² = 0.49
Experimental Δδ (ppm)
Calculated Δδ (ppm)

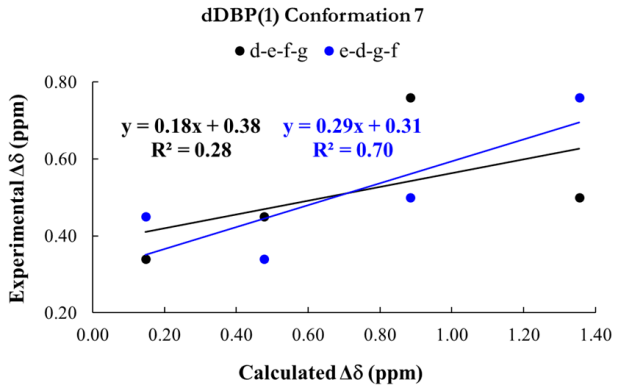

dDBP(1) Conformation 2
d-e-f-g
e-d-g-f
y = -0.10x + 0.60
R² = 0.11
y = 0.27x + 0.29
R² = 0.75
Experimental Δδ (ppm)
Calculated Δδ (ppm)

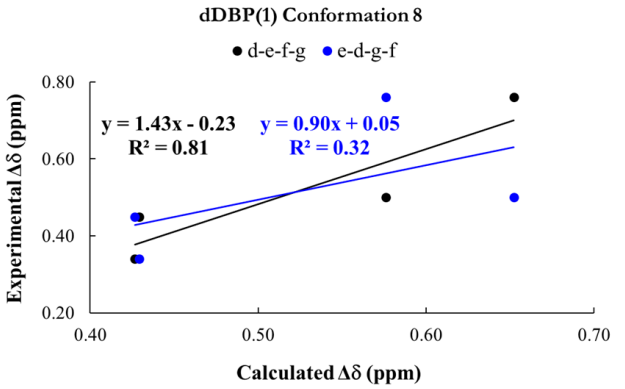

dDBP(1) Conformation 3
d-e-f-g
e-d-g-f
y = 0.26x + 0.39
R² = 0.95
y = 0.06x + 0.48
R² = 0.06
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(1) Conformation 4
d-e-f-g
e-d-g-f
y = 0.26x + 0.38
R² = 0.68
y = -0.10x + 0.56
R² = 0.09
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(1) Conformation 5
d-e-f-g
e-d-g-f
y = 1.62x - 0.41
R² = 0.92
y = 0.61x + 0.17
R² = 0.13
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(1) Conformation 6
d-e-f-g
e-d-g-f
y = 1.38x - 0.29
R² = 0.59
y = 1.36x - 0.28
R² = 0.57
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(1) Conformation 7
d-e-f-g
e-d-g-f
y = 0.18x + 0.38
R² = 0.28
y = 0.29x + 0.31
R² = 0.70
Experimental Δδ (ppm)
Calculated Δδ (ppm)


dDBP(1) Conformation 8
d-e-f-g
e-d-g-f
y = 1.43x - 0.23
R² = 0.81
y = 0.90x + 0.05
R² = 0.32
Experimental Δδ (ppm)
Calculated Δδ (ppm)

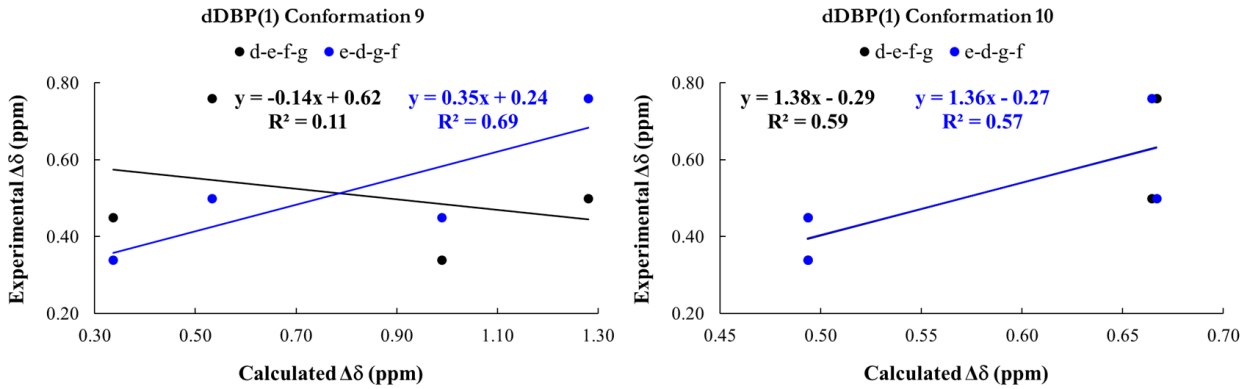


Figure S63. Experimental Δδ *versus* calculated Δδ NMR plots for each of the 10 folded conformations analyzed for **dDBP(1)**. The title of each plot refers to the conformation number in Table S10 and Figure S62.

dDBP(hyd,1)

Twelve conformations were analyzed for **dDBP(hyd,1)** (truncated version of **dDBP(hyd,6)**). For all 12 conformers, the *ortho* methoxy group is initially set planar to the DBP core, with the methyl group pointing away from the ester (steric bulk prevents the methoxy group from pointing towards the ester). This configuration was found to be energetically favourable according to calculations of **DBP(1)**. The 12 conformations arise from the following geometrical factors: there are four starting configurations between the two esters and the phenyl linker – the dihedral angle between both carbonyls is 0° (**+3/2**), 90° (**+1/2**), 180° (**-1/2**), or 270° (**-3/2**). There are three starting configurations between the two esters and the DBP core – both carbonyls are syn (**+1**), one carbonyl is syn and the other is anti (**0**), or both carbonyls are anti (**-1**) to H(a) on the DBP core (see Figure S54 for schematic of the DBP core. A seen below, the conformers are all very close in energy.

Table S11. The total number of conformations, energies, relative energies, and number of imaginary frequencies for each conformer of **dDBP(hyd,1)**.

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	(**+3/2**, **+1**)	-3509.3745	+0.5	0
2	(**+3/2**, **0**)	-3509.3747	+0.4	1
3	(**+3/2**, **-1**)	-3509.3745	+0.5	0
4	(**+1/2**, **+1**)	-3509.3746	+0.4	0
5	(**+1/2**, **0**)	-3509.3748	+0.3	0
6	(**+1/2**, **-1**)	-3509.3748	+0.3	0
7	(**-1/2**, **+1**)	-3509.3753	0.0	1
8	(**-1/2**, **0**)	-3509.3752	+0.1	1
9	(**-1/2**, **-1**)	-3509.3752	0.0	0
10	(**-3/2**, **+1**)	-3509.3751	+0.1	0
11	(**-3/2**, **0**)	-3509.3751	+0.1	1
12	(**-3/2**, **-1**)	-3509.3751	+0.1	0

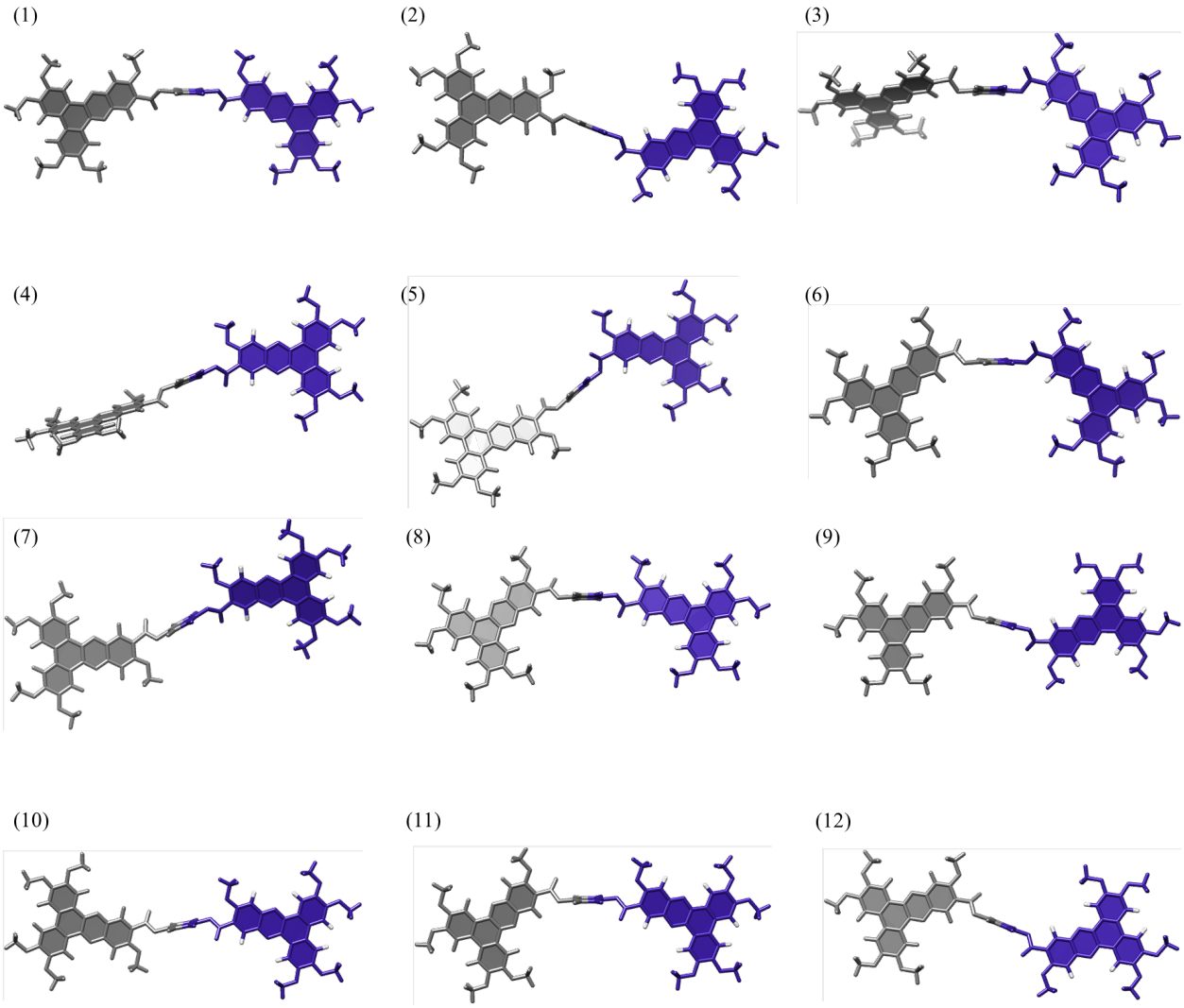


Figure S64. Schematics of all 12 conformations for **dDBP(hyd,1)**. The number displayed in the figure corresponds to the conformation number in Table S11. For each conformation, the DBP core on the right is coloured in violet and the other DBP core is coloured in grey. Hydrogens on the DBP core in violet are shown in light grey.

V. Cartesian Coordinates

The cartesian coordinates are included for the lowest energy structure (folded and unfolded, where applicable) of each compound. In addition, for dimers that can fold, the cartesian coordinates of the folded conformer with the best R^2 in the experimental $\Delta\delta$ *versus* calculated $\Delta\delta$ plots are included below.

DBP(Me,H) – lowest energy conformation (#2 in Table S5).

```
0 1
 C                  4.58360000   -2.28410000   -0.00370000
 C                  3.26410000   -2.64570000   -0.00850000
 C                  2.25300000   -1.65260000   -0.00480000
 C                  2.63040000   -0.27220000    0.00420000
 C                  3.99930000    0.07540000    0.00870000
 C                  4.96020000   -0.91380000    0.00490000
 H                  5.37240000   -3.02910000   -0.00630000
 H                  2.95820000   -3.68750000   -0.01530000
 H                  4.26610000    1.12620000    0.01560000
 C                  0.42310000    0.33990000    0.00560000
 C                  0.04270000   -1.05080000   -0.00590000
 C                 -0.60250000    1.36540000    0.01880000
 C                 -1.96320000    1.00390000   -0.00460000
 C                 -0.22820000    2.72260000    0.02180000
 C                 -2.92060000    2.03880000   -0.00930000
 C                 -1.17450000    3.72240000    0.01430000
 H                  0.83070000    2.94680000    0.03080000
 C                 -2.55150000    3.37030000   -0.00160000
 H                 -3.97350000    1.79500000   -0.02620000
 C                 -1.36090000   -1.40980000   -0.01840000
 C                 -2.34810000   -0.40470000    0.00930000
 C                 -1.73040000   -2.76910000   -0.02420000
 C                 -3.69840000   -0.80760000    0.01700000
 C                 -3.05350000   -3.14690000   -0.01500000
 H                 -0.93290000   -3.50080000   -0.03660000
 C                 -4.05870000   -2.14170000    0.00690000
 H                 -4.48080000   -0.06220000    0.03790000
 N                  0.95550000   -2.01540000   -0.01150000
 N                  1.69790000    0.70350000    0.01070000
 O                 -3.50840000   -4.42510000   -0.02210000
 O                 -5.33300000   -2.60230000    0.01700000
 O                 -3.41330000    4.41670000   -0.00920000
 O                 -0.91300000    5.05380000    0.01810000
 C                 -2.52730000   -5.45850000   -0.04780000
 H                 -1.90520000   -5.39310000   -0.95020000
 H                 -1.88450000   -5.41850000    0.84160000
 H                 -3.08530000   -6.39590000   -0.05440000
 C                 -6.38370000   -1.64240000    0.04450000
 H                 -7.31010000   -2.21860000    0.05070000
 H                 -6.33320000   -1.02200000    0.94950000
```

H	-6.35950000	-0.99910000	-0.84550000
C	-4.80630000	4.12560000	-0.02550000
H	-5.08670000	3.56590000	-0.92820000
H	-5.10620000	3.55990000	0.86720000
H	-5.31030000	5.09320000	-0.02780000
C	0.45870000	5.44050000	0.03080000
H	0.45850000	6.53150000	0.03210000
H	0.96720000	5.07060000	0.93080000
H	0.98290000	5.07280000	-0.86120000
C	6.41260000	-0.60770000	0.01000000
O	7.28790000	-1.44790000	0.00830000
O	6.66180000	0.72190000	0.01670000
C	8.05900000	1.07330000	0.02180000
H	8.08470000	2.16330000	0.02590000
H	8.55100000	0.67110000	0.91190000
H	8.55580000	0.67760000	-0.86860000

DBP(1) – lowest energy conformation (#1 in Table S6).

0 1

C	0.53890000	-1.04570000	-0.00670000
C	2.75020000	-1.63950000	-0.00600000
C	3.12950000	-0.25920000	0.00630000
C	0.91620000	0.33930000	0.00590000
H	3.46700000	-3.67270000	-0.02120000
C	3.76710000	-2.62910000	-0.01150000
C	4.50000000	0.09820000	0.01320000
C	5.45530000	-0.89360000	0.00790000
H	4.74240000	1.15420000	0.02300000
C	-0.86480000	-1.41140000	-0.01880000
C	-1.85530000	-0.41060000	0.00790000
C	-1.23120000	-2.77100000	-0.02500000
C	-3.20580000	-0.81740000	0.01480000
C	-2.55390000	-3.15220000	-0.01670000
H	-0.43210000	-3.50080000	-0.03710000
C	-3.56250000	-2.15140000	0.00460000
H	-3.98980000	-0.07350000	0.03520000
C	-0.11170000	1.36180000	0.01830000
C	0.25830000	2.72080000	0.02170000
C	-1.47250000	0.99760000	-0.00570000
C	-0.68990000	3.71810000	0.01370000
H	1.31680000	2.94650000	0.03130000
C	-2.43190000	2.03150000	-0.01100000
C	-2.06610000	3.36340000	-0.00300000
H	-3.48420000	1.78480000	-0.02890000
N	2.19370000	0.70980000	0.01310000
N	1.45780000	-2.00710000	-0.01360000
O	6.79880000	-0.68340000	0.01420000
C	7.24740000	0.66930000	0.02950000
H	6.90540000	1.20910000	-0.86330000

```
 H                  6.89650000    1.19150000    0.92920000
 H                  8.33740000    0.62300000    0.03440000
 O                 -3.00420000   -4.43360000   -0.02420000
 O                 -4.83770000   -2.61720000    0.01410000
 O                 -0.43100000    5.05180000    0.01770000
 O                 -2.93100000    4.40880000   -0.01120000
 C                 -2.01880000   -5.46180000   -0.05010000
 H                 -1.39590000   -5.39310000   -0.95180000
 H                 -1.37610000   -5.41980000    0.83940000
 H                 -2.57210000   -6.40220000   -0.05780000
 C                 -5.88820000   -1.65880000    0.04030000
 H                 -6.81480000   -2.23480000    0.04580000
 H                 -5.83940000   -1.03680000    0.94470000
 H                 -5.86390000   -1.01480000   -0.84960000
 C                 -4.32240000    4.11280000   -0.02830000
 H                 -4.62110000    3.54510000    0.86360000
 H                 -4.83030000    5.07840000   -0.03050000
 H                 -4.60060000    3.55190000   -0.93110000
 C                  0.93930000    5.43930000    0.03100000
 H                  1.44840000    5.06930000    0.93100000
 H                  1.46490000    5.07170000   -0.86050000
 H                  0.93900000    6.53040000    0.03240000
 C                  5.08350000   -2.26720000   -0.00490000
 H                  5.87660000   -3.00840000   -0.00890000
```

DBP(PrOH,H) – lowest energy conformation (#2 in Table S7).

```
0 1
 C                 -0.39120000    0.08960000   -0.00180000
 C                  1.65890000   -0.93220000    0.00120000
 C                  1.02530000   -2.21540000    0.00380000
 C                 -1.02970000   -1.20330000    0.00340000
 H                  3.53100000    0.12940000   -0.00070000
 C                  3.06880000   -0.85150000    0.00130000
 C                  1.82900000   -3.38260000    0.00580000
 C                  3.19340000   -3.27870000    0.00570000
 C                  3.82390000   -2.00520000    0.00350000
 H                  1.33150000   -4.34780000    0.00780000
 H                  3.82540000   -4.16070000    0.00750000
 C                 -1.20220000    1.29210000   -0.01320000
 C                 -2.60680000    1.19630000    0.00850000
 C                 -0.57640000    2.55340000   -0.01350000
 C                 -3.34980000    2.39430000    0.01370000
 C                 -1.31510000    3.71500000   -0.00530000
 H                  0.50580000    2.57310000   -0.02120000
 C                 -2.73420000    3.63140000    0.00840000
 H                 -4.42980000    2.35530000    0.02800000
 C                 -2.47600000   -1.28810000    0.01340000
 C                 -3.09870000   -2.55180000    0.01270000
```

```
 C                  -3.25310000   -0.11290000   -0.00850000
 C                  -4.46970000   -2.66990000    0.00350000
 H                  -2.45680000   -3.42320000    0.02070000
 C                  -4.65550000   -0.25040000   -0.01440000
 C                  -5.26450000   -1.49100000   -0.00990000
 H                  -5.28110000    0.63080000   -0.02850000
 C                   5.30820000   -1.97950000    0.00360000
 O                   6.00850000   -2.97090000    0.00560000
 O                   5.80250000   -0.72110000    0.00130000
 O                  -5.16050000   -3.83770000    0.00400000
 O                  -6.60340000   -1.69930000   -0.01800000
 O                  -0.80590000    4.97230000   -0.00690000
 O                  -3.38170000    4.82230000    0.01600000
 C                   7.24500000   -0.62390000    0.00130000
 H                   7.63590000   -1.13870000    0.88780000
 H                   7.63620000   -1.14200000   -0.88310000
 C                   7.59250000    0.85000000   -0.00140000
 H                   7.16180000    1.33320000   -0.88620000
 H                   7.16180000    1.33650000    0.88160000
 C                   9.09700000    1.05880000   -0.00180000
 H                   9.54260000    0.58700000    0.89010000
 H                   9.54260000    0.58380000   -0.89200000
 O                   9.33390000    2.46740000   -0.00440000
 H                  10.28530000    2.61340000   -0.00450000
 N                  -0.31760000   -2.32420000    0.00640000
 N                   0.92960000    0.20350000   -0.00330000
 C                   0.61410000    5.09370000   -0.01950000
 H                   1.06070000    4.63380000    0.87200000
 H                   1.04470000    4.63620000   -0.92010000
 H                   0.81910000    6.16520000   -0.01990000
 C                  -4.80460000    4.80030000    0.03190000
 H                  -5.18540000    4.30130000    0.93340000
 H                  -5.11650000    5.84570000    0.03630000
 H                  -5.20550000    4.30280000   -0.86170000
 C                  -7.45090000   -0.55570000   -0.02990000
 H                  -7.28840000    0.05160000   -0.93060000
 H                  -8.47050000   -0.94350000   -0.03280000
 H                  -7.29770000    0.06290000    0.86480000
 C                  -4.39510000   -5.03960000    0.01470000
 H                  -3.75840000   -5.11340000   -0.87690000
 H                  -3.77030000   -5.10540000    0.91530000
 H                  -5.12210000   -5.85300000    0.01350000
```

DBP(PrOH,1) – lowest energy conformation (#1 in Table S8).

```
0 1
 C                  -5.94330000    0.54830000   -2.88450000
 C                  -5.70960000    0.71870000   -5.15390000
 C                  -6.94960000    0.03450000   -5.34410000
```

C	-7.19090000	-0.14430000	-3.07310000
H	-4.04270000	1.65950000	-6.14930000
C	-4.98380000	1.13730000	-6.28870000
C	-7.42830000	-0.19080000	-6.65400000
C	-6.69790000	0.22440000	-7.74740000
C	-5.43480000	0.88580000	-7.56400000
H	-8.38620000	-0.68640000	-6.75230000
C	-7.94020000	-0.59380000	-1.91750000
C	-9.16390000	-1.26750000	-2.10110000
C	-7.46340000	-0.32930000	-0.61770000
C	-9.91260000	-1.69120000	-1.02730000
H	-9.48860000	-1.43730000	-3.11950000
C	-8.24090000	-0.77230000	0.47160000
C	-9.43860000	-1.43640000	0.28850000
H	-7.90260000	-0.58680000	1.48130000
C	-5.45570000	0.80440000	-1.54240000
C	-6.18720000	0.35260000	-0.42740000
C	-4.23240000	1.47770000	-1.36270000
C	-5.66220000	0.61080000	0.85570000
C	-3.73060000	1.71960000	-0.10360000
H	-3.70490000	1.79690000	-2.25230000
C	-4.46350000	1.27500000	1.03010000
H	-6.20040000	0.27860000	1.73230000
N	-7.67240000	-0.38890000	-4.28840000
N	-5.22740000	0.96560000	-3.92150000
C	-4.54440000	1.34550000	-8.66970000
O	-3.77270000	2.27570000	-8.55820000
O	-4.63790000	0.58920000	-9.77890000
O	-7.12080000	0.08580000	-9.02510000
C	-8.38450000	-0.53560000	-9.24330000
H	-8.39050000	-1.56600000	-8.86520000
H	-9.19480000	0.03480000	-8.77070000
H	-8.52390000	-0.54330000	-10.32530000
O	-2.56540000	2.35940000	0.16950000
O	-3.89530000	1.55380000	2.23020000
O	-10.23900000	-1.88620000	1.28610000
O	-11.09910000	-2.34710000	-1.10270000
C	-9.81850000	-1.65440000	2.62590000
H	-8.86000000	-2.14890000	2.83430000
H	-9.73190000	-0.57980000	2.83670000
H	-10.59510000	-2.08700000	3.25840000
C	-11.60320000	-2.61570000	-2.40740000
H	-12.54840000	-3.13980000	-2.25750000
H	-11.78130000	-1.68620000	-2.96430000
H	-10.91440000	-3.25450000	-2.97620000
C	-4.58740000	1.13420000	3.40000000
H	-3.96840000	1.45190000	4.24040000
H	-5.57440000	1.61120000	3.47220000
H	-4.70400000	0.04200000	3.42520000
C	-1.80250000	2.81330000	-0.94530000
H	-1.49840000	1.97560000	-1.58670000
H	-2.36510000	3.54310000	-1.54240000

```
 H                 -0.91730000    3.29090000   -0.52280000
 C                 -3.76900000    0.98010000  -10.86680000
 H                 -2.72580000    0.90510000  -10.53470000
 H                 -3.96300000    2.03010000  -11.11800000
 C                 -4.06780000    0.05100000  -12.02530000
 H                 -3.88950000   -0.98820000  -11.72570000
 H                 -5.12430000    0.13540000  -12.30490000
 C                 -3.20280000    0.38040000  -13.22920000
 H                 -2.13650000    0.28990000  -12.96200000
 H                 -3.38270000    1.42080000  -13.54830000
 O                 -3.54690000   -0.53710000  -14.26900000
 H                 -3.00340000   -0.33880000  -15.03830000
```

dDBP(H) – lowest energy folded conformation (#5 in Table S9).

```
0 1
 C                  0.19300000    0.14390000    1.75930000
 C                  2.40080000    0.74020000    1.69870000
 C                  2.02940000    2.11450000    1.55900000
 C                 -0.18240000    1.53000000    1.63290000
 H                  4.04350000   -0.66000000    1.79440000
 C                  3.76560000    0.38420000    1.68930000
 C                  3.04520000    3.09100000    1.41510000
 C                  4.36090000    2.71600000    1.35670000
 C                  4.72820000    1.34980000    1.49380000
 H                  2.75040000    4.13400000    1.34430000
 H                  5.13750000    3.45950000    1.21920000
 C                 -0.83170000   -0.87820000    1.80780000
 C                 -2.19230000   -0.52010000    1.76340000
 C                 -0.45290000   -2.23180000    1.86500000
 C                 -3.14830000   -1.55480000    1.79860000
 C                 -1.39680000   -3.23070000    1.86340000
 H                  0.60630000   -2.45420000    1.87000000
 C                 -2.77430000   -2.88350000    1.84260000
 H                 -4.20230000   -1.31850000    1.75620000
 C                 -1.58590000    1.88730000    1.57990000
 C                 -1.95300000    3.23460000    1.40830000
 C                 -2.57280000    0.88180000    1.63110000
 C                 -3.27480000    3.60670000    1.30180000
 H                 -1.15610000    3.96460000    1.34360000
 C                 -3.92070000    1.27830000    1.53430000
 C                 -4.27720000    2.60380000    1.37520000
 H                 -4.70070000    0.53090000    1.57380000
 C                  6.14220000    0.91090000    1.39150000
 O                  6.56700000   -0.15770000    1.77320000
 O                  6.89820000    1.86060000    0.78750000
 O                 -3.72410000    4.87210000    1.10940000
 O                 -5.55570000    3.05480000    1.25610000
 O                 -1.12980000   -4.56280000    1.85530000
```

O	-3.62970000	-3.93410000	1.84410000
C	8.29220000	1.55670000	0.56150000
H	8.80480000	2.51580000	0.68220000
H	8.64090000	0.85580000	1.32770000
C	8.53100000	1.00820000	-0.83870000
H	8.02090000	1.63820000	-1.57780000
H	9.60800000	1.09690000	-1.03700000
C	8.16880000	-0.44980000	-1.04300000
H	8.61080000	-0.83690000	-1.96900000
H	8.52330000	-1.06910000	-0.21220000
O	6.72880000	-0.58100000	-1.14060000
N	0.73380000	2.48650000	1.54550000
N	1.46550000	-0.22450000	1.80420000
C	0.24700000	-4.93590000	1.78050000
H	0.71290000	-4.52140000	0.87730000
H	0.79770000	-4.59770000	2.66770000
H	0.25570000	-6.02640000	1.74030000
C	-5.02700000	-3.65580000	1.78960000
H	-5.29280000	-3.12900000	0.86470000
H	-5.52020000	-4.62890000	1.79810000
H	-5.34690000	-3.07460000	2.66520000
C	-6.60230000	2.09620000	1.34380000
H	-6.59180000	1.57990000	2.31300000
H	-7.53100000	2.65970000	1.24130000
H	-6.53470000	1.35370000	0.53530000
C	-2.73230000	5.88670000	0.93520000
H	-2.11890000	5.99590000	1.83930000
H	-2.09440000	5.66490000	0.07060000
H	-3.28710000	6.80980000	0.75950000
C	6.29280000	-1.86130000	-1.09400000
O	7.04180000	-2.81380000	-1.02490000
C	4.28500000	-3.29930000	-1.01820000
C	2.93590000	-3.51800000	-1.06260000
C	2.04320000	-2.43160000	-1.23250000
C	2.57120000	-1.10750000	-1.35640000
C	3.97100000	-0.90750000	-1.31150000
C	4.81390000	-1.98580000	-1.14310000
H	4.98510000	-4.11850000	-0.89380000
H	2.52030000	-4.51850000	-0.98480000
H	4.35290000	0.10330000	-1.40890000
C	0.44440000	-0.27740000	-1.55190000
C	-0.08510000	-1.61460000	-1.45230000
N	0.71600000	-2.66000000	-1.28860000
N	1.75060000	-0.04750000	-1.50810000
C	-0.46440000	0.84460000	-1.68250000
C	0.04800000	2.15530000	-1.69900000
C	-1.85250000	0.62410000	-1.77510000
C	-0.78980000	3.24210000	-1.78800000
H	1.11970000	2.27270000	-1.60280000
C	-2.69380000	1.74680000	-1.90320000
C	-2.18960000	3.03180000	-1.90640000
H	-3.76450000	1.61480000	-1.96700000

```
 C                 -1.51680000   -1.82870000   -1.53330000
 C                 -2.03610000   -3.13110000   -1.41140000
 C                 -2.38530000   -0.73030000   -1.69020000
 C                 -3.39250000   -3.36730000   -1.45760000
 H                 -1.33090000   -3.93930000   -1.26520000
 C                 -3.76890000   -0.98810000   -1.75120000
 C                 -4.27320000   -2.26900000   -1.64040000
 H                 -4.46000000   -0.16610000   -1.87450000
 O                 -3.98750000   -4.57890000   -1.32620000
 O                 -5.59650000   -2.58730000   -1.67200000
 O                 -2.93510000    4.16050000   -1.99400000
 O                 -0.39800000    4.54290000   -1.75460000
 C                 -3.13260000   -5.68870000   -1.04220000
 H                 -2.43430000   -5.86870000   -1.87030000
 H                 -2.57890000   -5.52630000   -0.10920000
 H                 -3.79630000   -6.54820000   -0.93430000
 C                 -6.52250000   -1.52580000   -1.86400000
 H                 -6.35270000   -1.01430000   -2.82090000
 H                 -7.51020000   -1.98960000   -1.86910000
 H                 -6.46670000   -0.79290000   -1.04570000
 C                 -4.34980000    4.01560000   -2.09860000
 H                 -4.76490000    3.50920000   -1.21860000
 H                 -4.74660000    5.03070000   -2.14430000
 H                 -4.62230000    3.47230000   -3.01370000
 C                  0.99750000    4.78220000   -1.57600000
 H                  1.57740000    4.38860000   -2.42110000
 H                  1.10860000    5.86690000   -1.53030000
 H                  1.35290000    4.32750000   -0.64330000
```

dDBP(H) – folded conformation that best fit the ^{1}H-NMR data (#10 in Table S9).

```
0 1
 C                  0.24070000   -0.83160000   -1.47780000
 C                  2.19100000    0.36390000   -1.58950000
 C                  1.44680000    1.56270000   -1.82470000
 C                 -0.50690000    0.37770000   -1.71430000
 H                  4.14790000   -0.49450000   -1.32950000
 C                  3.60070000    0.42320000   -1.51550000
 C                  2.13980000    2.78720000   -1.99300000
 C                  3.50500000    2.81910000   -1.91670000
 C                  4.24620000    1.63200000   -1.66590000
 H                  1.55350000    3.68240000   -2.17990000
 H                  4.05680000    3.74460000   -2.04730000
 C                 -0.46540000   -2.08510000   -1.29680000
 C                 -1.86960000   -2.12540000   -1.39870000
 C                  0.26270000   -3.26190000   -1.04170000
 C                 -2.50720000   -3.37100000   -1.23850000
 C                 -0.37450000   -4.47190000   -0.88150000
 H                  1.33990000   -3.17640000   -0.97000000
```

C	-1.79060000	-4.52530000	-0.98860000
H	-3.58460000	-3.43480000	-1.30290000
C	-1.95280000	0.33000000	-1.76420000
C	-2.67730000	1.52360000	-1.93300000
C	-2.62670000	-0.89710000	-1.61290000
C	-4.05260000	1.52210000	-1.94540000
H	-2.10820000	2.43960000	-2.02560000
C	-4.03390000	-0.88560000	-1.65690000
C	-4.74440000	0.28820000	-1.82080000
H	-4.58360000	-1.80830000	-1.53410000
C	5.72250000	1.76340000	-1.58540000
O	6.32740000	2.78190000	-1.85410000
O	6.32720000	0.62880000	-1.16560000
O	-4.83540000	2.63060000	-2.05800000
O	-6.09900000	0.37570000	-1.85470000
O	0.23860000	-5.65720000	-0.63510000
O	-2.34040000	-5.75670000	-0.82250000
C	7.77230000	0.69530000	-1.08480000
H	8.17090000	0.71340000	-2.10640000
H	8.06010000	1.63450000	-0.59800000
C	8.27760000	-0.51370000	-0.32130000
H	7.83980000	-1.43410000	-0.72430000
H	9.36090000	-0.57960000	-0.49060000
C	8.06280000	-0.45160000	1.18420000
H	8.55570000	-1.29570000	1.67680000
H	8.44540000	0.48840000	1.59480000
O	6.66030000	-0.45090000	1.53070000
N	0.10280000	1.54380000	-1.88820000
N	1.56650000	-0.82070000	-1.42180000
C	1.66510000	-5.65710000	-0.63610000
H	2.05830000	-5.32950000	-1.60740000
H	2.06850000	-5.00930000	0.15260000
H	1.96070000	-6.69050000	-0.44890000
C	-3.73660000	-5.89200000	-1.06900000
H	-3.98700000	-5.58880000	-2.09450000
H	-3.95850000	-6.95200000	-0.93590000
H	-4.33370000	-5.30390000	-0.35890000
C	-6.84030000	-0.83710000	-1.72680000
H	-6.64200000	-1.32370000	-0.76270000
H	-7.89060000	-0.54580000	-1.78380000
H	-6.60960000	-1.52760000	-2.54890000
C	-4.15960000	3.85920000	-2.31780000
H	-3.45500000	4.11020000	-1.51310000
H	-3.61260000	3.81400000	-3.26880000
H	-4.93910000	4.62070000	-2.37810000
C	6.05440000	-1.66020000	1.53240000
O	6.64580000	-2.71040000	1.37970000
C	3.86570000	-2.75620000	1.94980000
C	2.50350000	-2.73580000	2.07330000
C	1.79500000	-1.51530000	1.94250000
C	2.52320000	-0.30310000	1.73000000
C	3.93100000	-0.34490000	1.63970000

```
C                  4.58950000   -1.55330000    1.72790000
H                  4.42580000   -3.68340000    2.01820000
H                  1.92880000   -3.63910000    2.25660000
H                  4.46750000    0.58030000    1.46110000
C                  0.55870000    0.86560000    1.61170000
C                 -0.17350000   -0.35920000    1.81840000
N                  0.45100000   -1.51630000    1.99990000
N                  1.88440000    0.87610000    1.57910000
C                 -0.16310000    2.10830000    1.41780000
C                  0.55230000    3.30060000    1.20340000
C                 -1.57100000    2.11820000    1.44470000
C                 -0.10100000    4.49710000    1.01150000
H                  1.63290000    3.23690000    1.18230000
C                 -2.22550000    3.35370000    1.26930000
C                 -1.52110000    4.52440000    1.06320000
H                 -3.30580000    3.39820000    1.30100000
C                 -1.61960000   -0.34050000    1.80420000
C                 -2.32650000   -1.55130000    1.91980000
C                 -2.30980000    0.87100000    1.60310000
C                 -3.69830000   -1.58320000    1.83170000
H                 -1.74480000   -2.45550000    2.04670000
C                 -3.71510000    0.82550000    1.54370000
C                 -4.40630000   -0.36630000    1.64690000
H                 -4.27570000    1.73390000    1.37370000
O                 -4.46080000   -2.70930000    1.89310000
O                 -5.75610000   -0.48440000    1.56580000
O                 -2.08510000    5.74980000    0.90180000
O                  0.49970000    5.69280000    0.78580000
C                 -3.78580000   -3.91260000    2.25920000
H                 -3.03380000   -4.19670000    1.51170000
H                 -3.30040000   -3.80670000    3.23830000
H                 -4.55910000   -4.68100000    2.31570000
C                 -6.52020000    0.71930000    1.48380000
H                 -6.30990000    1.26860000    0.55710000
H                 -7.56500000    0.40320000    1.48660000
H                 -6.33130000    1.36120000    2.35420000
C                 -3.47930000    5.87290000    1.16250000
H                 -3.72160000    5.53260000    2.17820000
H                 -3.70520000    6.93620000    1.06760000
H                 -4.08280000    5.31030000    0.43710000
C                  1.92630000    5.70710000    0.78920000
H                  2.33500000    5.05440000    0.00700000
H                  2.21170000    6.74140000    0.59190000
H                  2.32200000    5.39440000    1.76450000
```

dDBP(H) – extended, unfolded conformation (#11 in Table S9).

```
0 1
C                  8.94090000  -18.89410000   -7.87160000
```

C	9.30300000	-17.02030000	-6.60530000
C	8.95870000	-16.19360000	-7.72180000
C	8.59760000	-18.06070000	-8.99800000
H	9.93120000	-17.04490000	-4.53720000
C	9.66870000	-16.41780000	-5.38330000
C	8.99070000	-14.78510000	-7.57390000
C	9.35050000	-14.22310000	-6.37800000
C	9.69460000	-15.04400000	-5.26900000
H	8.72540000	-14.17480000	-8.43200000
H	9.37730000	-13.14550000	-6.26570000
C	8.90790000	-20.33760000	-8.00940000
C	8.57270000	-20.92140000	-9.24620000
C	9.24770000	-21.14850000	-6.90970000
C	8.57840000	-22.32820000	-9.33460000
C	9.24960000	-22.52150000	-7.01110000
H	9.50640000	-20.65000000	-5.98450000
C	8.90760000	-23.12270000	-8.25310000
H	8.32710000	-22.80820000	-10.26990000
C	8.23770000	-18.67420000	-10.25990000
C	7.89460000	-17.85900000	-11.35640000
C	8.20080000	-20.07780000	-10.37870000
C	7.52960000	-18.40710000	-12.56470000
H	7.93080000	-16.78730000	-11.20950000
C	7.82750000	-20.62380000	-11.62300000
C	7.49610000	-19.82220000	-12.69900000
H	7.78950000	-21.69670000	-11.74770000
C	10.09640000	-14.46900000	-3.96010000
O	10.39360000	-15.11790000	-2.98010000
O	10.09870000	-13.11380000	-3.97990000
O	7.18440000	-17.70830000	-13.67540000
O	7.12520000	-20.27570000	-13.92070000
O	9.55870000	-23.38420000	-6.01140000
O	8.93790000	-24.47780000	-8.26450000
C	10.49280000	-12.48030000	-2.74300000
H	9.80630000	-12.79170000	-1.94620000
H	11.49790000	-12.82430000	-2.46970000
C	10.44800000	-10.98420000	-2.98370000
H	11.11390000	-10.72590000	-3.81540000
H	9.43200000	-10.68620000	-3.26820000
C	10.87270000	-10.22840000	-1.74010000
H	10.21750000	-10.43700000	-0.88510000
H	11.89900000	-10.47200000	-1.43960000
O	10.79580000	-8.82180000	-2.05990000
N	8.61110000	-16.73620000	-8.90520000
N	9.28360000	-18.36650000	-6.70500000
C	9.91150000	-22.81400000	-4.75320000
H	10.80470000	-22.18160000	-4.84040000
H	9.08460000	-22.22200000	-4.33940000
H	10.12290000	-23.65810000	-4.09520000
C	8.61040000	-25.13600000	-9.48310000
H	9.31060000	-24.86300000	-10.28420000
H	8.69570000	-26.20350000	-9.27480000

H	7.58310000	-24.90610000	-9.79710000
C	7.06940000	-21.68480000	-14.11470000
H	6.33630000	-22.15100000	-13.44260000
H	6.75540000	-21.82830000	-15.14950000
H	8.05430000	-22.14730000	-13.96430000
C	7.20120000	-16.28700000	-13.57330000
H	6.49450000	-15.93530000	-12.81000000
H	8.20760000	-15.91720000	-13.33620000
H	6.89650000	-15.91650000	-14.55310000
C	11.18180000	-7.98160000	-1.06890000
O	11.56670000	-8.36650000	0.01430000
C	10.58690000	-6.17320000	-2.75370000
C	10.49850000	-4.85010000	-3.09600000
C	10.89530000	-3.84580000	-2.17930000
C	11.39080000	-4.23160000	-0.89320000
C	11.46920000	-5.60080000	-0.56260000
C	11.07550000	-6.55700000	-1.47460000
H	10.28340000	-6.94140000	-3.45540000
H	10.12620000	-4.53770000	-4.06710000
H	11.84260000	-5.89280000	0.41380000
C	11.69510000	-2.02950000	-0.34180000
C	11.18810000	-1.64060000	-1.63510000
N	10.80080000	-2.54690000	-2.52490000
N	11.78620000	-3.30530000	0.00570000
C	12.12180000	-1.01070000	0.59830000
C	12.61440000	-1.39290000	1.86060000
C	12.01310000	0.35210000	0.26040000
C	13.01090000	-0.45260000	2.78470000
H	12.66900000	-2.45280000	2.07340000
C	12.42560000	1.30310000	1.21550000
C	12.91340000	0.92620000	2.45230000
H	12.35770000	2.35740000	0.98720000
C	11.09000000	-0.23560000	-1.97360000
C	10.59510000	0.14210000	-3.23730000
C	11.51750000	0.74440000	-1.05580000
C	10.50600000	1.46630000	-3.60060000
H	10.28890000	-0.65000000	-3.90830000
C	11.41790000	2.09620000	-1.44170000
C	10.92770000	2.46470000	-2.68030000
H	11.73550000	2.87270000	-0.76010000
O	10.04290000	1.92820000	-4.78950000
O	10.80630000	3.74040000	-3.12000000
O	13.32430000	1.78200000	3.41980000
O	13.49860000	-0.72100000	4.02140000
C	9.60660000	0.95380000	-5.73320000
H	10.42610000	0.28060000	-6.01750000
H	8.77040000	0.36280000	-5.33650000
H	9.27510000	1.51630000	-6.60730000
C	11.22110000	4.78440000	-2.24570000
H	12.28960000	4.70180000	-2.00530000
H	11.04200000	5.71320000	-2.78900000
H	10.63320000	4.78490000	-1.31780000

```
 C                 13.25110000    3.17620000    3.14430000
 H                 12.21600000    3.49230000    2.95640000
 H                 13.62510000    3.67450000    4.03990000
 H                 13.88100000    3.44690000    2.28600000
 C                 13.60560000   -2.09460000    4.38800000
 H                 14.28700000   -2.63310000    3.71640000
 H                 14.01020000   -2.09930000    5.40100000
 H                 12.62330000   -2.58510000    4.38070000
```

dDBP(1) – lowest energy folded conformation (#6 in Table S10).

```
0 1
 C                  0.49900000    0.49730000    1.59990000
 C                  2.65610000   -0.25670000    1.50200000
 C                  2.19400000   -1.60610000    1.44480000
 C                  0.03130000   -0.86380000    1.57880000
 H                  4.37880000    1.02370000    1.51830000
 C                  4.04410000   -0.00610000    1.48100000
 C                  3.13510000   -2.65730000    1.35950000
 C                  4.48700000   -2.38580000    1.32880000
 C                  4.95990000   -1.02950000    1.38200000
 H                  2.74780000   -3.66850000    1.33740000
 C                 -1.39120000   -1.12830000    1.66580000
 C                 -1.85990000   -2.45600000    1.60980000
 C                 -2.30160000   -0.05890000    1.78930000
 C                 -3.20530000   -2.73730000    1.67110000
 H                 -1.12320000   -3.24070000    1.49670000
 C                 -3.67350000   -0.36650000    1.87170000
 C                 -4.12700000   -1.66680000    1.81170000
 H                 -4.39450000    0.43470000    1.94910000
 C                 -0.45310000    1.58850000    1.65840000
 C                 -1.82680000    1.31930000    1.80230000
 C                  0.00490000    2.91570000    1.58340000
 C                 -2.70970000    2.41290000    1.89830000
 C                 -0.87260000    3.97360000    1.65280000
 H                  1.06860000    3.06780000    1.45300000
 C                 -2.25860000    3.71640000    1.82870000
 H                 -3.77170000    2.24150000    2.00290000
 N                  0.87690000   -1.88760000    1.49310000
 N                  1.79650000    0.77690000    1.56740000
 C                  6.40580000   -0.70420000    1.25210000
 O                  7.24180000   -1.37610000    0.69050000
 O                  6.68090000    0.48980000    1.83830000
 O                  5.44310000   -3.34340000    1.28230000
 C                  5.01990000   -4.70280000    1.26400000
 H                  4.45740000   -4.95780000    2.17180000
 H                  4.40270000   -4.91650000    0.38090000
 H                  5.93590000   -5.29390000    1.22140000
 O                 -0.52870000    5.28640000    1.55180000
```

O	-3.04850000	4.81790000	1.88780000
O	-5.43740000	-2.03440000	1.85900000
O	-3.76170000	-3.97330000	1.59420000
C	-6.39980000	-1.00220000	2.02960000
H	-6.24170000	-0.45970000	2.97130000
H	-6.37370000	-0.28940000	1.19300000
H	-7.37100000	-1.50010000	2.05510000
C	-2.86680000	-5.07590000	1.46500000
H	-3.49830000	-5.96150000	1.38340000
H	-2.25480000	-4.98340000	0.56020000
H	-2.21690000	-5.15840000	2.34660000
C	-4.45670000	4.61590000	1.98830000
H	-4.89590000	5.61480000	1.99620000
H	-4.84070000	4.05980000	1.12390000
H	-4.71540000	4.09680000	2.92140000
C	0.85040000	5.57250000	1.32870000
H	1.47000000	5.21980000	2.16340000
H	1.20560000	5.11600000	0.39510000
H	0.91960000	6.65900000	1.25600000
C	8.01300000	1.00970000	1.63160000
H	8.74820000	0.23410000	1.87320000
H	8.08690000	1.82070000	2.36290000
C	8.24500000	1.53740000	0.21950000
H	9.19320000	2.09090000	0.23560000
H	8.36470000	0.70450000	-0.48050000
C	7.15660000	2.46130000	-0.29870000
H	7.49090000	3.02610000	-1.17590000
H	6.81750000	3.18070000	0.45840000
O	6.04830000	1.61720000	-0.68330000
C	5.00780000	2.21920000	-1.28640000
O	4.94870000	3.41470000	-1.48820000
C	3.90540000	1.26380000	-1.59500000
C	2.63410000	1.78660000	-1.58280000
C	1.49840000	0.96100000	-1.72170000
C	1.68880000	-0.44610000	-1.89100000
C	2.99680000	-0.97020000	-1.97520000
C	4.09050000	-0.14420000	-1.83280000
H	2.49520000	2.84990000	-1.41610000
H	3.09570000	-2.03670000	-2.13480000
C	-0.57880000	-0.74950000	-1.84610000
C	-0.76780000	0.66760000	-1.70430000
N	0.63470000	-1.28080000	-1.96080000
N	0.26740000	1.49780000	-1.65520000
C	-1.72800000	-1.62920000	-1.83180000
C	-1.53620000	-3.01710000	-1.96460000
C	-3.02240000	-1.10370000	-1.65120000
C	-2.59730000	-3.88920000	-1.90040000
H	-0.52060000	-3.36500000	-2.10310000
C	-4.09260000	-2.01480000	-1.54540000
C	-3.90150000	-3.37950000	-1.66140000
H	-5.09200000	-1.64980000	-1.35050000
C	-2.11040000	1.20850000	-1.61710000

```
 C                 -2.29220000    2.60110000   -1.54930000
 C                 -3.21680000    0.33940000   -1.55030000
 C                 -3.54850000    3.14800000   -1.42010000
 H                 -1.40700000    3.22340000   -1.58210000
 C                 -4.49760000    0.91440000   -1.42120000
 C                 -4.67250000    2.28310000   -1.35070000
 H                 -5.36930000    0.27470000   -1.38520000
 O                 -2.51000000   -5.24320000   -2.02010000
 O                 -4.87400000   -4.31580000   -1.55800000
 O                 -5.87500000    2.91040000   -1.21900000
 O                 -3.82700000    4.47410000   -1.34210000
 C                 -2.72310000    5.37570000   -1.44880000
 H                 -3.15590000    6.37550000   -1.39070000
 H                 -2.01520000    5.24060000   -0.62290000
 H                 -2.20860000    5.25000000   -2.41050000
 C                 -7.04400000    2.10390000   -1.25520000
 H                 -7.88580000    2.79550000   -1.19080000
 H                 -7.10780000    1.53430000   -2.19210000
 H                 -7.08140000    1.40840000   -0.40450000
 C                 -6.17040000   -3.87760000   -1.15800000
 H                 -6.77350000   -4.78330000   -1.07620000
 H                 -6.12620000   -3.37230000   -0.18470000
 H                 -6.61600000   -3.21460000   -1.91270000
 C                 -1.21310000   -5.78060000   -2.25690000
 H                 -0.78810000   -5.39740000   -3.19420000
 H                 -0.52680000   -5.54860000   -1.43030000
 H                 -1.34770000   -6.86110000   -2.32960000
 O                  5.36640000   -0.57290000   -1.92310000
 C                  5.59420000   -1.96480000   -2.14540000
 H                  5.15310000   -2.56780000   -1.34300000
 H                  5.18930000   -2.27610000   -3.11740000
 H                  6.67680000   -2.08860000   -2.12580000
```

dDBP(1) – folded conformation that best fit the ^{1}H-NMR data (#2 in Table S10).

```
0 1
 C                 -0.11880000   -0.33390000    1.69400000
 C                  2.07460000   -0.97260000    1.58930000
 C                  1.67930000   -2.34060000    1.47760000
 C                 -0.51900000   -1.70610000    1.53590000
 H                  3.75680000    0.38220000    1.62320000
 C                  3.45140000   -0.65770000    1.55790000
 C                  2.66520000   -3.35100000    1.40080000
 C                  4.00090000   -3.01630000    1.36770000
 C                  4.40160000   -1.63860000    1.40960000
 H                  2.32380000   -4.37910000    1.38850000
 C                 -1.92690000   -2.03380000    1.44310000
 C                 -2.31400000   -3.36210000    1.18690000
 C                 -2.89680000   -1.01570000    1.53950000
```

C	-3.63920000	-3.70320000	1.03640000
H	-1.52820000	-4.09990000	1.08780000
C	-4.25000000	-1.38190000	1.39780000
C	-4.62600000	-2.68900000	1.15500000
H	-5.01710000	-0.62290000	1.46300000
C	-1.12600000	0.70090000	1.81620000
C	-2.49310000	0.36770000	1.76020000
C	-0.72830000	2.04220000	1.96540000
C	-3.43390000	1.41090000	1.87370000
C	-1.65850000	3.05180000	2.04190000
H	0.33400000	2.24930000	1.97780000
C	-3.04050000	2.72770000	2.00530000
H	-4.49150000	1.19130000	1.83020000
N	0.37710000	-2.68390000	1.44960000
N	1.16400000	0.00960000	1.71130000
C	5.82110000	-1.19450000	1.29750000
O	6.28760000	-0.26360000	1.91580000
O	6.49000000	-1.92600000	0.38430000
O	5.00450000	-3.92670000	1.35020000
C	4.64660000	-5.30470000	1.35670000
H	4.07780000	-5.56470000	2.25920000
H	4.06050000	-5.56730000	0.46570000
H	5.58900000	-5.85420000	1.34710000
O	-1.37270000	4.37830000	2.13140000
O	-3.88190000	3.78860000	2.08550000
O	-5.91020000	-3.11030000	0.98940000
O	-4.10530000	-4.94700000	0.75690000
C	-6.94110000	-2.14080000	1.12210000
H	-6.93260000	-1.68090000	2.11930000
H	-6.85260000	-1.35430000	0.35850000
H	-7.87830000	-2.68100000	0.97790000
C	-3.12490000	-5.96260000	0.53450000
H	-3.68850000	-6.86350000	0.28590000
H	-2.46510000	-5.69200000	-0.29950000
H	-2.53180000	-6.14170000	1.44120000
C	-5.28200000	3.53190000	2.01140000
H	-5.76370000	4.50860000	2.07790000
H	-5.55150000	3.06540000	1.05570000
H	-5.61230000	2.90220000	2.84900000
C	0.00880000	4.73400000	2.09440000
H	0.54550000	4.32910000	2.96260000
H	0.47640000	4.37190000	1.17030000
H	0.03410000	5.82490000	2.12690000
C	7.88740000	-1.63160000	0.17020000
H	8.38820000	-2.60520000	0.19790000
H	8.25940000	-1.00510000	0.98770000
C	8.09820000	-0.96990000	-1.18230000
H	9.15890000	-1.08590000	-1.44400000
H	7.52270000	-1.50520000	-1.94750000
C	7.79790000	0.51330000	-1.23790000
H	8.11890000	0.94220000	-2.19390000
H	8.31510000	1.05540000	-0.43650000

O	6.37410000	0.72080000	-1.08790000
C	5.99600000	2.01960000	-1.22400000
O	6.78370000	2.90610000	-1.46520000
C	4.52410000	2.18680000	-1.08940000
C	3.67730000	1.12930000	-1.34040000
C	2.27360000	1.29070000	-1.33160000
C	1.73130000	2.58680000	-1.07600000
C	2.59930000	3.66130000	-0.78530000
C	3.96510000	3.47530000	-0.77160000
H	4.07930000	0.14730000	-1.56590000
H	2.14970000	4.62620000	-0.58590000
C	-0.38380000	1.75570000	-1.35860000
C	0.16240000	0.43980000	-1.56070000
N	0.40070000	2.79940000	-1.11020000
N	1.47430000	0.23270000	-1.56200000
C	-1.81740000	1.95490000	-1.42830000
C	-2.35320000	3.23910000	-1.21690000
C	-2.67150000	0.85850000	-1.66180000
C	-3.71190000	3.46070000	-1.24880000
H	-1.65730000	4.04220000	-1.01120000
C	-4.05810000	1.10380000	-1.71110000
C	-4.57830000	2.36760000	-1.51210000
H	-4.73870000	0.28410000	-1.89440000
C	-0.73070000	-0.68760000	-1.74550000
C	-0.20250000	-1.98980000	-1.82090000
C	-2.12150000	-0.48130000	-1.82750000
C	-1.02710000	-3.08160000	-1.96670000
H	0.87010000	-2.10040000	-1.72400000
C	-2.94800000	-1.60630000	-2.01950000
C	-2.42780000	-2.88250000	-2.08990000
H	-4.02020000	-1.48420000	-2.07970000
O	-4.32180000	4.65330000	-1.03110000
O	-5.90570000	2.67200000	-1.52600000
O	-3.15950000	-4.01420000	-2.24840000
O	-0.61970000	-4.37830000	-1.98890000
C	0.77830000	-4.61020000	-1.82590000
H	0.90110000	-5.69480000	-1.83930000
H	1.35160000	-4.16640000	-2.65070000
H	1.13510000	-4.20370000	-0.87110000
C	-4.57130000	-3.87630000	-2.38820000
H	-4.95530000	-4.89050000	-2.50860000
H	-5.02130000	-3.43000000	-1.49290000
H	-4.82170000	-3.27990000	-3.27630000
C	-6.81770000	1.61600000	-1.79760000
H	-7.81100000	2.06750000	-1.77660000
H	-6.63650000	1.17430000	-2.78660000
H	-6.75760000	0.82890000	-1.03190000
C	-3.47860000	5.74950000	-0.67180000
H	-2.92140000	5.52960000	0.24750000
H	-2.78250000	5.99310000	-1.48560000
H	-4.15090000	6.59280000	-0.50530000
O	4.84530000	4.44350000	-0.44530000

```
 C                  4.32930000    5.72180000   -0.08970000
 H                  3.78310000    6.17720000   -0.92600000
 H                  3.67040000    5.65430000    0.78680000
 H                  5.20100000    6.33120000    0.15180000
```

dDBP(1) – extended, unfolded conformation (#11 in Table S10).

```
0 1
 C                  6.74710000  -17.69790000    8.91430000
 C                  7.16140000  -16.29990000    7.15150000
 C                  6.06990000  -15.46490000    7.54250000
 C                  5.64350000  -16.86170000    9.30770000
 H                  8.73830000  -16.58260000    5.70610000
 C                  7.91330000  -15.94660000    6.01110000
 C                  5.76050000  -14.31680000    6.77880000
 C                  6.51690000  -13.98840000    5.67420000
 C                  7.63090000  -14.80990000    5.29060000
 H                  4.90720000  -13.72820000    7.09270000
 C                  4.85440000  -17.21960000   10.46890000
 C                  3.77460000  -16.40120000   10.85550000
 C                  5.18510000  -18.36290000   11.22410000
 C                  3.01290000  -16.70240000   11.96090000
 H                  3.56950000  -15.52970000   10.24730000
 C                  4.39260000  -18.65930000   12.35140000
 C                  3.32940000  -17.85940000   12.72380000
 H                  4.61620000  -19.53100000   12.95020000
 C                  7.07300000  -18.87760000    9.69310000
 C                  6.29420000  -19.21940000   10.81510000
 C                  8.15150000  -19.69380000    9.30260000
 C                  6.64290000  -20.38240000   11.53200000
 C                  8.47750000  -20.82910000   10.01010000
 H                  8.71250000  -19.39410000    8.42680000
 C                  7.70510000  -21.17890000   11.15090000
 H                  6.06810000  -20.67110000   12.40080000
 N                  5.32320000  -15.76770000    8.62260000
 N                  7.48320000  -17.40500000    7.84940000
 C                  8.52620000  -14.53370000    4.13020000
 O                  9.06880000  -15.40640000    3.48590000
 O                  8.72360000  -13.21890000    3.91210000
 O                  6.24920000  -12.93480000    4.86690000
 C                  5.12190000  -12.12450000    5.18660000
 H                  4.19310000  -12.70940000    5.16490000
 H                  5.23700000  -11.65370000    6.17160000
 H                  5.08700000  -11.35340000    4.41560000
 O                  9.49560000  -21.67560000    9.71400000
 O                  8.09690000  -22.31130000   11.78730000
 O                  2.52540000  -18.08200000   13.79230000
 O                  1.95490000  -15.97940000   12.41040000
 C                  2.79030000  -19.22950000   14.59150000
```

H	2.69770000	-20.15380000	14.00520000
H	3.78980000	-19.17880000	15.04420000
H	2.03490000	-19.22190000	15.37860000
C	1.61140000	-14.81310000	11.66890000
H	0.75070000	-14.37970000	12.18060000
H	2.43740000	-14.08940000	11.66060000
H	1.33720000	-15.06450000	10.63560000
C	7.35680000	-22.71280000	12.93380000
H	7.82900000	-23.63200000	13.28390000
H	7.40450000	-21.95330000	13.72620000
H	6.30700000	-22.91490000	12.68090000
C	10.28650000	-21.35910000	8.57140000
H	9.67850000	-21.34880000	7.65720000
H	10.78460000	-20.38750000	8.68850000
H	11.03640000	-22.14850000	8.50340000
C	9.61530000	-12.90720000	2.81770000
H	9.19870000	-13.31970000	1.89030000
H	10.58320000	-13.39280000	2.99240000
C	9.73730000	-11.39720000	2.76770000
H	8.74590000	-10.94940000	2.63410000
H	10.14060000	-11.02820000	3.71760000
C	10.64640000	-10.97720000	1.62960000
H	10.25010000	-11.27710000	0.65180000
H	11.65240000	-11.40460000	1.72570000
O	10.73920000	-9.53580000	1.68030000
C	11.49770000	-8.97850000	0.71650000
O	12.07910000	-9.62490000	-0.12990000
C	11.61090000	-7.49580000	0.83360000
C	12.77490000	-6.94650000	0.34690000
C	13.03000000	-5.56220000	0.43390000
C	12.04330000	-4.71660000	1.02780000
C	10.83340000	-5.27770000	1.49400000
C	10.60910000	-6.63490000	1.40080000
H	13.52140000	-7.59250000	-0.10390000
H	10.10100000	-4.59710000	1.91020000
C	13.39630000	-2.90200000	0.67570000
C	14.38750000	-3.75610000	0.07500000
N	12.24790000	-3.38910000	1.13660000
N	14.19030000	-5.06410000	-0.03340000
C	13.64690000	-1.47890000	0.77750000
C	12.68110000	-0.64330000	1.37280000
C	14.86430000	-0.93970000	0.31490000
C	12.89400000	0.70940000	1.50630000
H	11.76720000	-1.10920000	1.71830000
C	15.06660000	0.44770000	0.45880000
C	14.11610000	1.26550000	1.03930000
H	15.98980000	0.89290000	0.11560000
C	15.62850000	-3.18750000	-0.41610000
C	16.58810000	-4.02440000	-1.01670000
C	15.85550000	-1.80130000	-0.32190000
C	17.76730000	-3.51460000	-1.51200000
H	16.36160000	-5.08130000	-1.07340000

```
 C                 17.06920000   -1.29440000   -0.83010000
 C                 18.01160000   -2.11780000   -1.41520000
 H                 17.27430000   -0.23460000   -0.77280000
 O                 12.02540000    1.59400000    2.06010000
 O                 14.24390000    2.60380000    1.21360000
 O                 19.19640000   -1.70290000   -1.92960000
 O                 18.74920000   -4.23810000   -2.10650000
 C                 18.53180000   -5.64120000   -2.23040000
 H                 19.41790000   -6.03450000   -2.73060000
 H                 18.42340000   -6.11590000   -1.24620000
 H                 17.64150000   -5.85330000   -2.83690000
 C                 19.49190000   -0.31280000   -1.86800000
 H                 20.47310000   -0.19810000   -2.33110000
 H                 18.75330000    0.27790000   -2.42710000
 H                 19.53530000    0.04110000   -0.82880000
 C                 15.44860000    3.21600000    0.76680000
 H                 15.34480000    4.27690000    0.99920000
 H                 16.32210000    2.80990000    1.29460000
 H                 15.58160000    3.09070000   -0.31640000
 C                 10.78980000    1.07010000    2.53650000
 H                 10.21470000    0.60620000    1.72400000
 H                 10.95090000    0.33350000    3.33510000
 H                 10.23920000    1.92460000    2.93300000
 O                  9.45420000   -7.22910000    1.78200000
 C                  8.42490000   -6.39880000    2.31230000
 H                  8.75580000   -5.89270000    3.22840000
 H                  8.09830000   -5.65190000    1.57700000
 H                  7.59740000   -7.07060000    2.54500000
```

dDBP(hyd,1) – lowest energy conformation (#9 in Table S11).

```
0 1
 C                  6.74710000  -17.69790000    8.91430000
 C                  7.16140000  -16.29990000    7.15150000
 C                  6.06990000  -15.46490000    7.54250000
 C                  5.64350000  -16.86170000    9.30770000
 H                  8.73830000  -16.58260000    5.70610000
 C                  7.91330000  -15.94660000    6.01110000
 C                  5.76050000  -14.31680000    6.77880000
 C                  6.51690000  -13.98840000    5.67420000
 C                  7.63090000  -14.80990000    5.29060000
 H                  4.90720000  -13.72820000    7.09270000
 C                  4.85440000  -17.21960000   10.46890000
 C                  3.77460000  -16.40120000   10.85550000
 C                  5.18510000  -18.36290000   11.22410000
 C                  3.01290000  -16.70240000   11.96090000
 H                  3.56950000  -15.52970000   10.24730000
 C                  4.39260000  -18.65930000   12.35140000
 C                  3.32940000  -17.85940000   12.72380000
```

H	4.61620000	-19.53100000	12.95020000
C	7.07300000	-18.87760000	9.69310000
C	6.29420000	-19.21940000	10.81510000
C	8.15150000	-19.69380000	9.30260000
C	6.64290000	-20.38240000	11.53200000
C	8.47750000	-20.82910000	10.01010000
H	8.71250000	-19.39410000	8.42680000
C	7.70510000	-21.17890000	11.15090000
H	6.06810000	-20.67110000	12.40080000
N	5.32320000	-15.76770000	8.62260000
N	7.48320000	-17.40500000	7.84940000
C	8.52620000	-14.53370000	4.13020000
O	9.06880000	-15.40640000	3.48590000
O	8.72360000	-13.21890000	3.91210000
O	6.24920000	-12.93480000	4.86690000
C	5.12190000	-12.12450000	5.18660000
H	4.19310000	-12.70940000	5.16490000
H	5.23700000	-11.65370000	6.17160000
H	5.08700000	-11.35340000	4.41560000
O	9.49560000	-21.67560000	9.71400000
O	8.09690000	-22.31130000	11.78730000
O	2.52540000	-18.08200000	13.79230000
O	1.95490000	-15.97940000	12.41040000
C	2.79030000	-19.22950000	14.59150000
H	2.69770000	-20.15380000	14.00520000
H	3.78980000	-19.17880000	15.04420000
H	2.03490000	-19.22190000	15.37860000
C	1.61140000	-14.81310000	11.66890000
H	0.75070000	-14.37970000	12.18060000
H	2.43740000	-14.08940000	11.66060000
H	1.33720000	-15.06450000	10.63560000
C	7.35680000	-22.71280000	12.93380000
H	7.82900000	-23.63200000	13.28390000
H	7.40450000	-21.95330000	13.72620000
H	6.30700000	-22.91490000	12.68090000
C	10.28650000	-21.35910000	8.57140000
H	9.67850000	-21.34880000	7.65720000
H	10.78460000	-20.38750000	8.68850000
H	11.03640000	-22.14850000	8.50340000
C	9.61530000	-12.90720000	2.81770000
H	9.19870000	-13.31970000	1.89030000
H	10.58320000	-13.39280000	2.99240000
C	9.73730000	-11.39720000	2.76770000
H	8.74590000	-10.94940000	2.63410000
H	10.14060000	-11.02820000	3.71760000
C	10.64640000	-10.97720000	1.62960000
H	10.25010000	-11.27710000	0.65180000
H	11.65240000	-11.40460000	1.72570000
O	10.73920000	-9.53580000	1.68030000
C	11.49770000	-8.97850000	0.71650000
O	12.07910000	-9.62490000	-0.12990000
C	11.61090000	-7.49580000	0.83360000

C	12.77490000	-6.94650000	0.34690000
C	13.03000000	-5.56220000	0.43390000
C	12.04330000	-4.71660000	1.02780000
C	10.83340000	-5.27770000	1.49400000
C	10.60910000	-6.63490000	1.40080000
H	13.52140000	-7.59250000	-0.10390000
H	10.10100000	-4.59710000	1.91020000
C	13.39630000	-2.90200000	0.67570000
C	14.38750000	-3.75610000	0.07500000
N	12.24790000	-3.38910000	1.13660000
N	14.19030000	-5.06410000	-0.03340000
C	13.64690000	-1.47890000	0.77750000
C	12.68110000	-0.64330000	1.37280000
C	14.86430000	-0.93970000	0.31490000
C	12.89400000	0.70940000	1.50630000
H	11.76720000	-1.10920000	1.71830000
C	15.06660000	0.44770000	0.45880000
C	14.11610000	1.26550000	1.03930000
H	15.98980000	0.89290000	0.11560000
C	15.62850000	-3.18750000	-0.41610000
C	16.58810000	-4.02440000	-1.01670000
C	15.85550000	-1.80130000	-0.32190000
C	17.76730000	-3.51460000	-1.51200000
H	16.36160000	-5.08130000	-1.07340000
C	17.06920000	-1.29440000	-0.83010000
C	18.01160000	-2.11780000	-1.41520000
H	17.27430000	-0.23460000	-0.77280000
O	12.02540000	1.59400000	2.06010000
O	14.24390000	2.60380000	1.21360000
O	19.19640000	-1.70290000	-1.92960000
O	18.74920000	-4.23810000	-2.10650000
C	18.53180000	-5.64120000	-2.23040000
H	19.41790000	-6.03450000	-2.73060000
H	18.42340000	-6.11590000	-1.24620000
H	17.64150000	-5.85330000	-2.83690000
C	19.49190000	-0.31280000	-1.86800000
H	20.47310000	-0.19810000	-2.33110000
H	18.75330000	0.27790000	-2.42710000
H	19.53530000	0.04110000	-0.82880000
C	15.44860000	3.21600000	0.76680000
H	15.34480000	4.27690000	0.99920000
H	16.32210000	2.80990000	1.29460000
H	15.58160000	3.09070000	-0.31640000
C	10.78980000	1.07010000	2.53650000
H	10.21470000	0.60620000	1.72400000
H	10.95090000	0.33350000	3.33510000
H	10.23920000	1.92460000	2.93300000
O	9.45420000	-7.22910000	1.78200000
C	8.42490000	-6.39880000	2.31230000
H	8.75580000	-5.89270000	3.22840000
H	8.09830000	-5.65190000	1.57700000
H	7.59740000	-7.07060000	2.54500000

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