

Supporting Information for

Semirigid Discotic Dimers: Flexible but not Flexible Enough?

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1. NMR Spectra

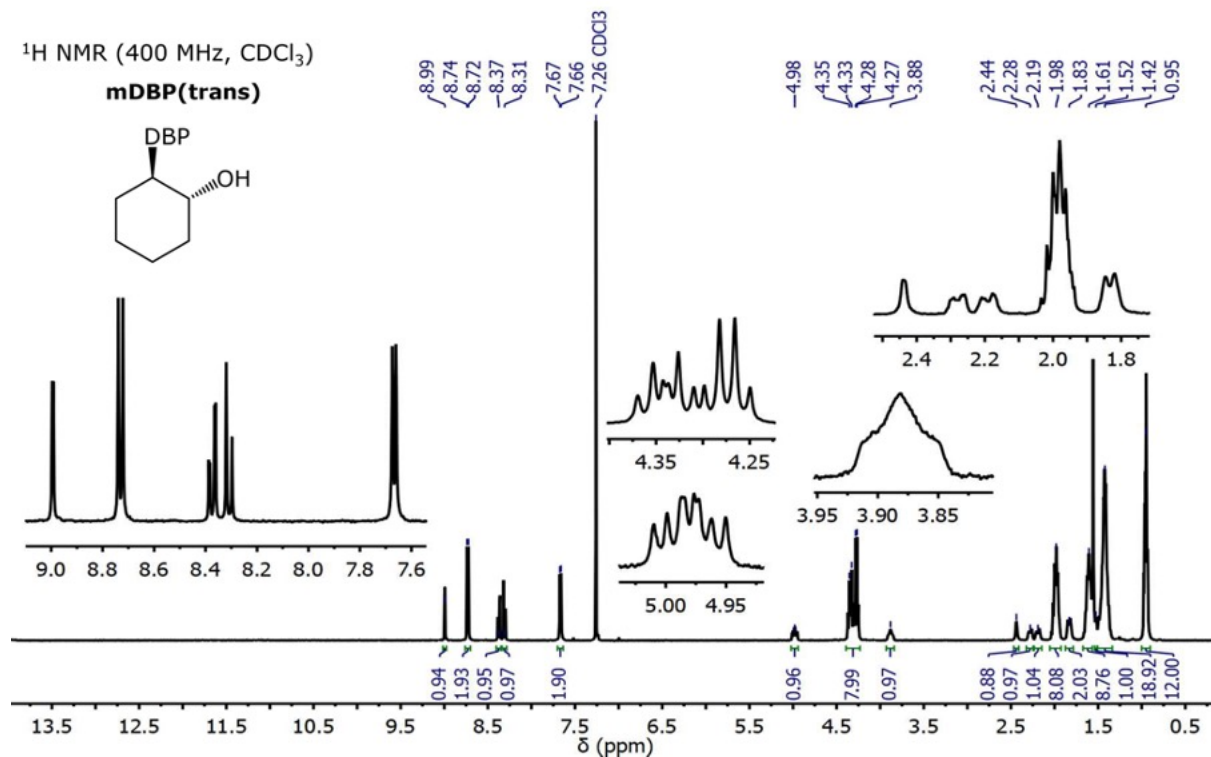


Figure S1. ¹H NMR spectrum of mDBP(trans).

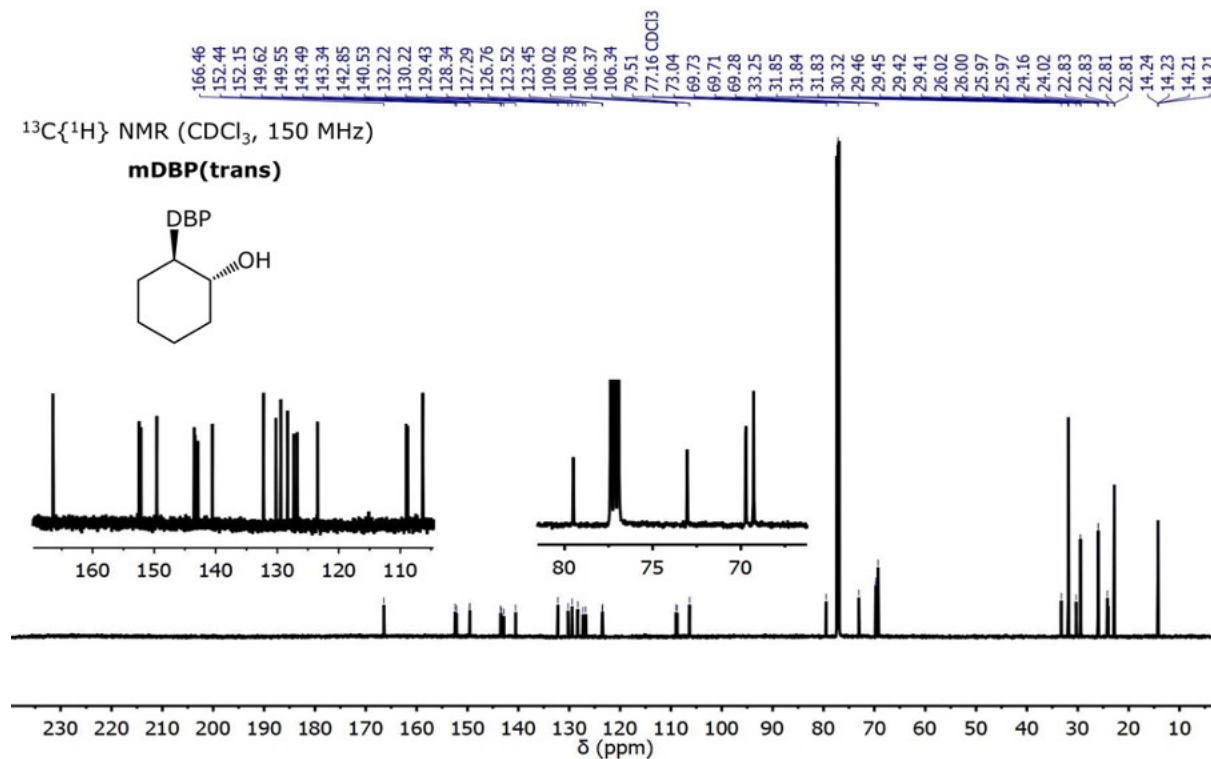


Figure S2. ¹³C{¹H} NMR spectrum of mDBP(trans).

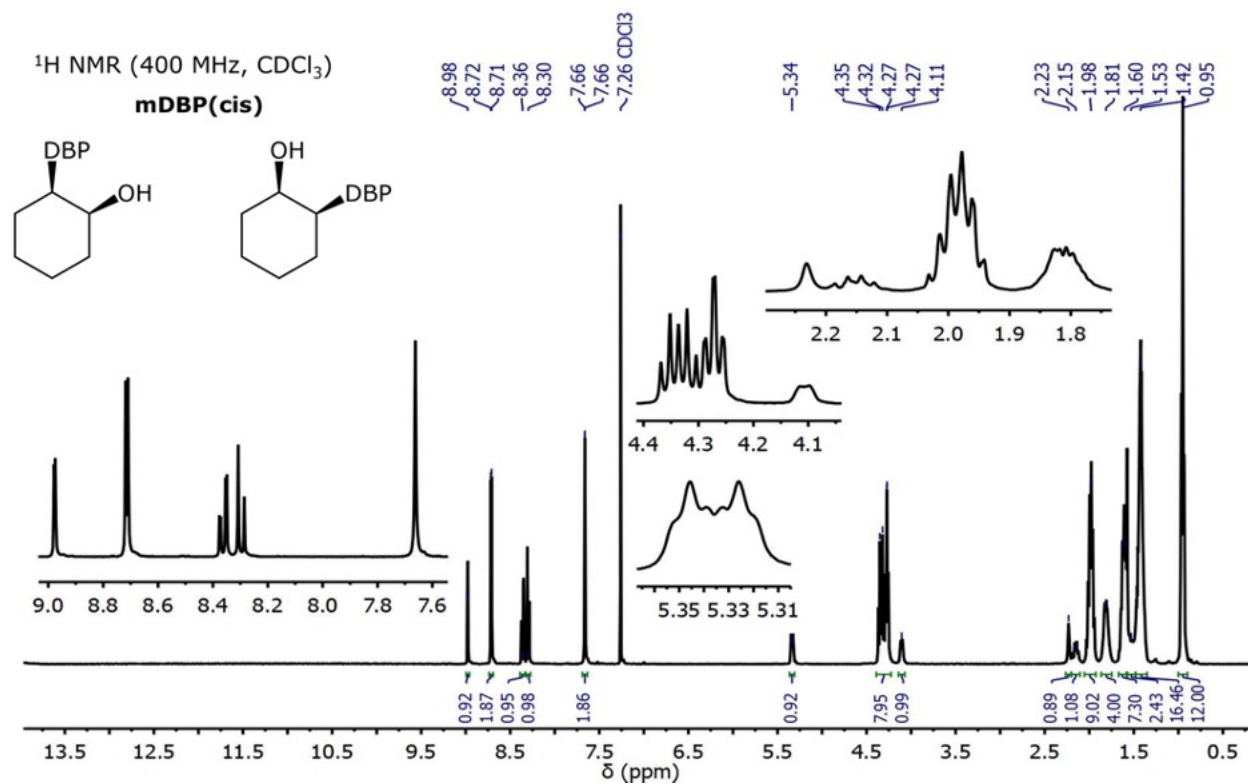


Figure S3. ¹H NMR spectrum of mDBP(cis).

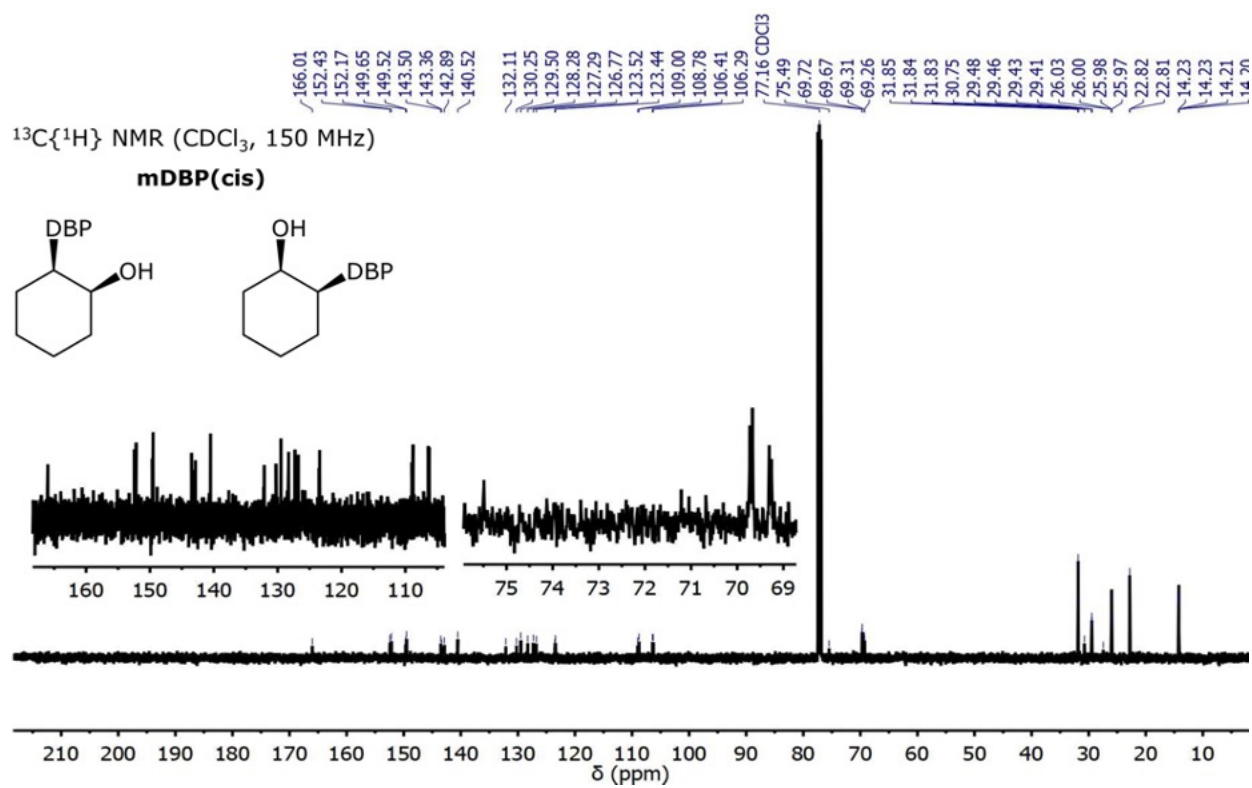


Figure S4. ¹³C{¹H} NMR spectrum of mDBP(cis).

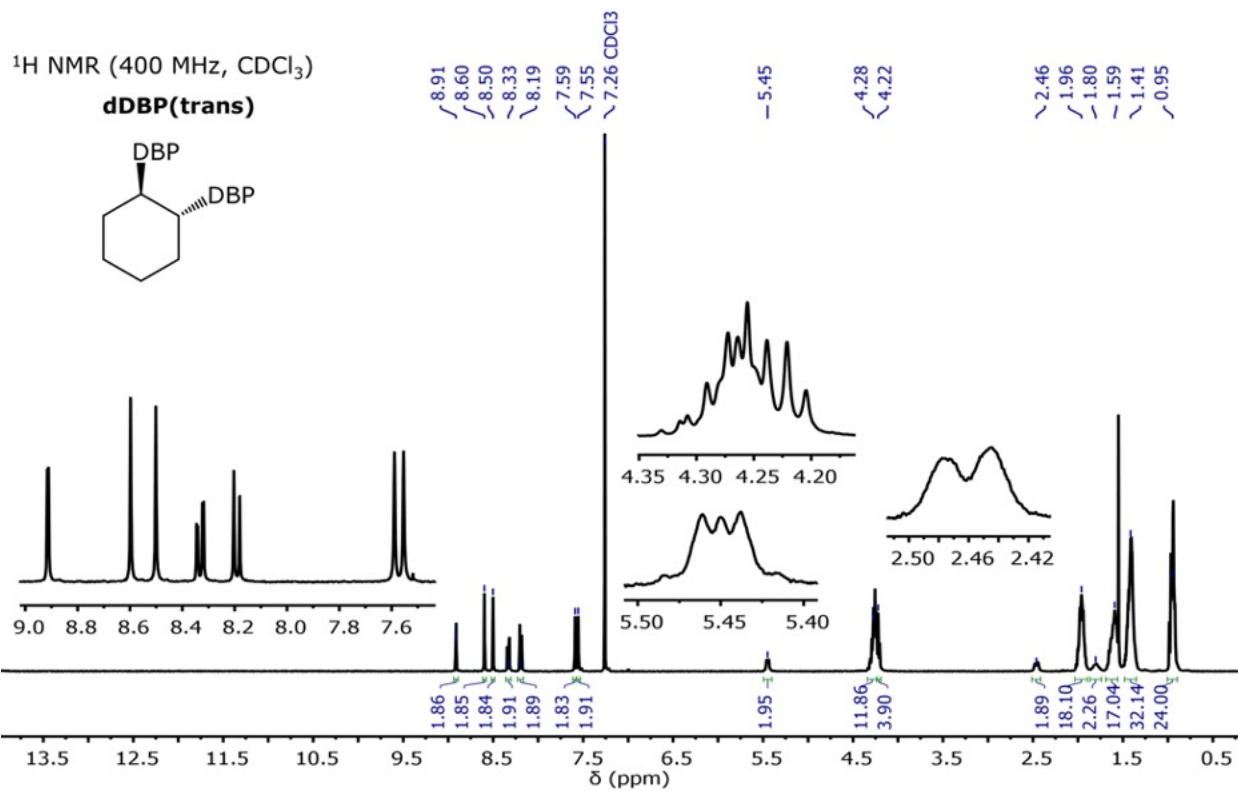


Figure S5. ¹H NMR spectrum of **dDBP(trans)**.

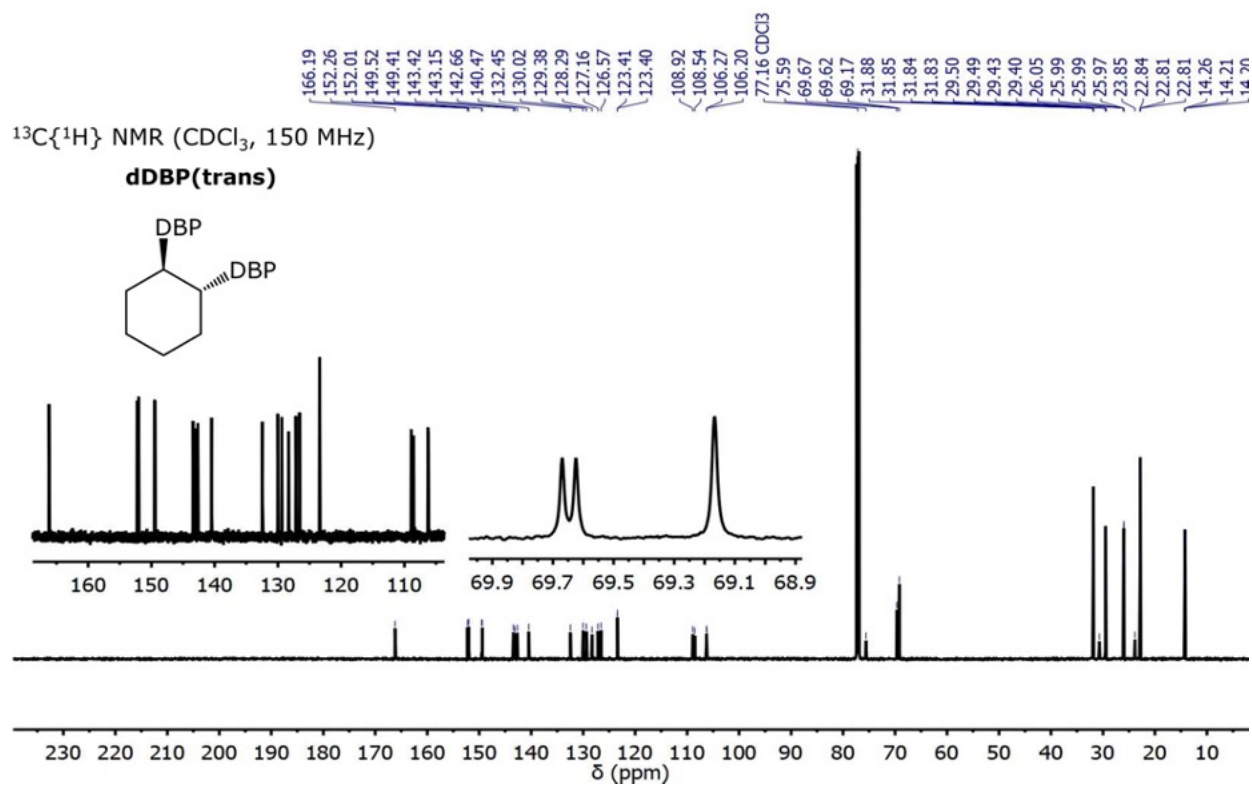


Figure S6. ¹³C{¹H} NMR spectrum of **dDBP(trans)**.

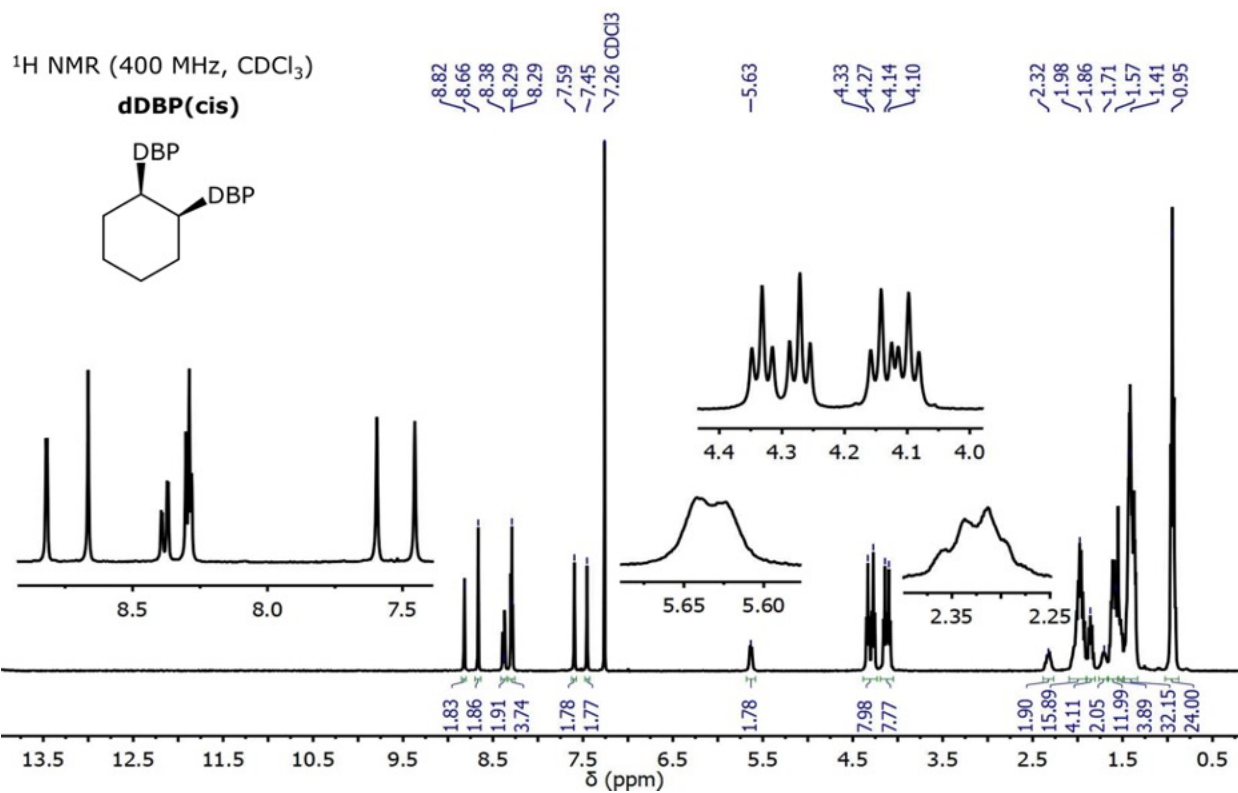


Figure S7. ^1H NMR spectrum of **dDBP(cis)**.

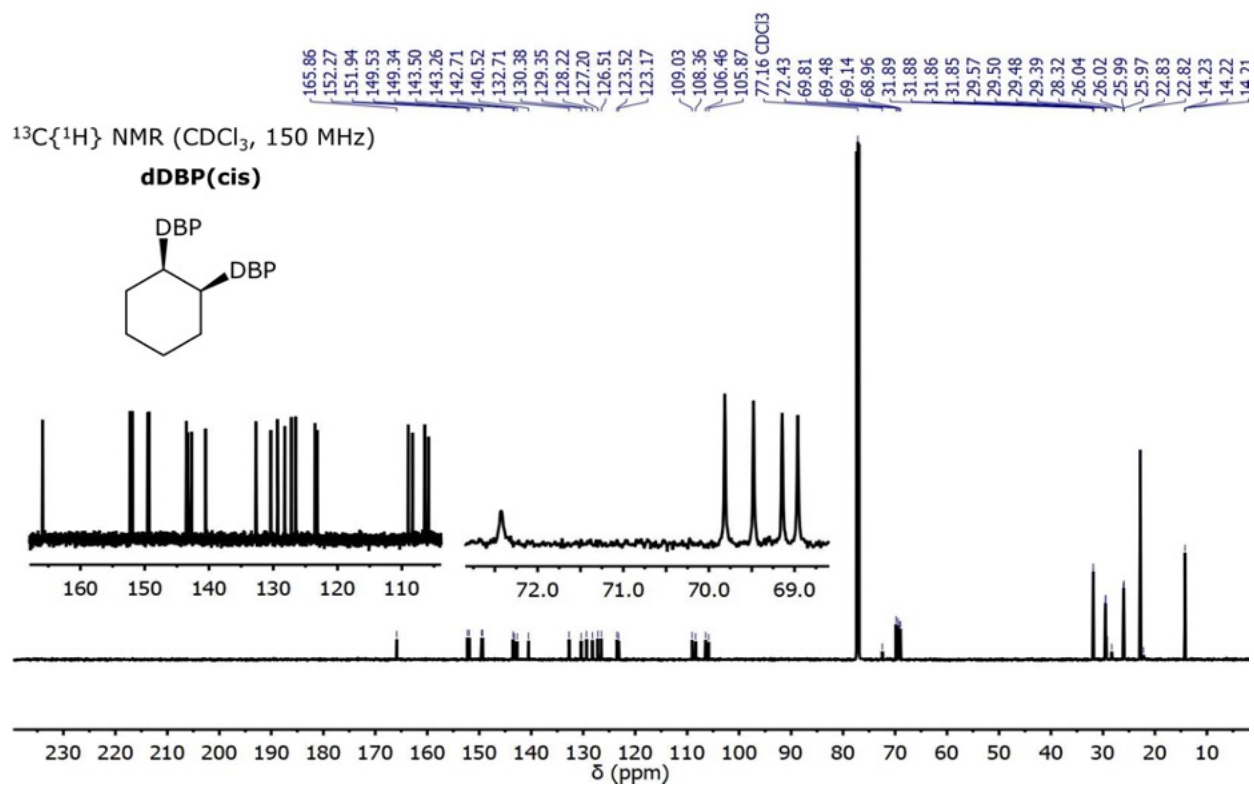


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **dDBP(cis)**.

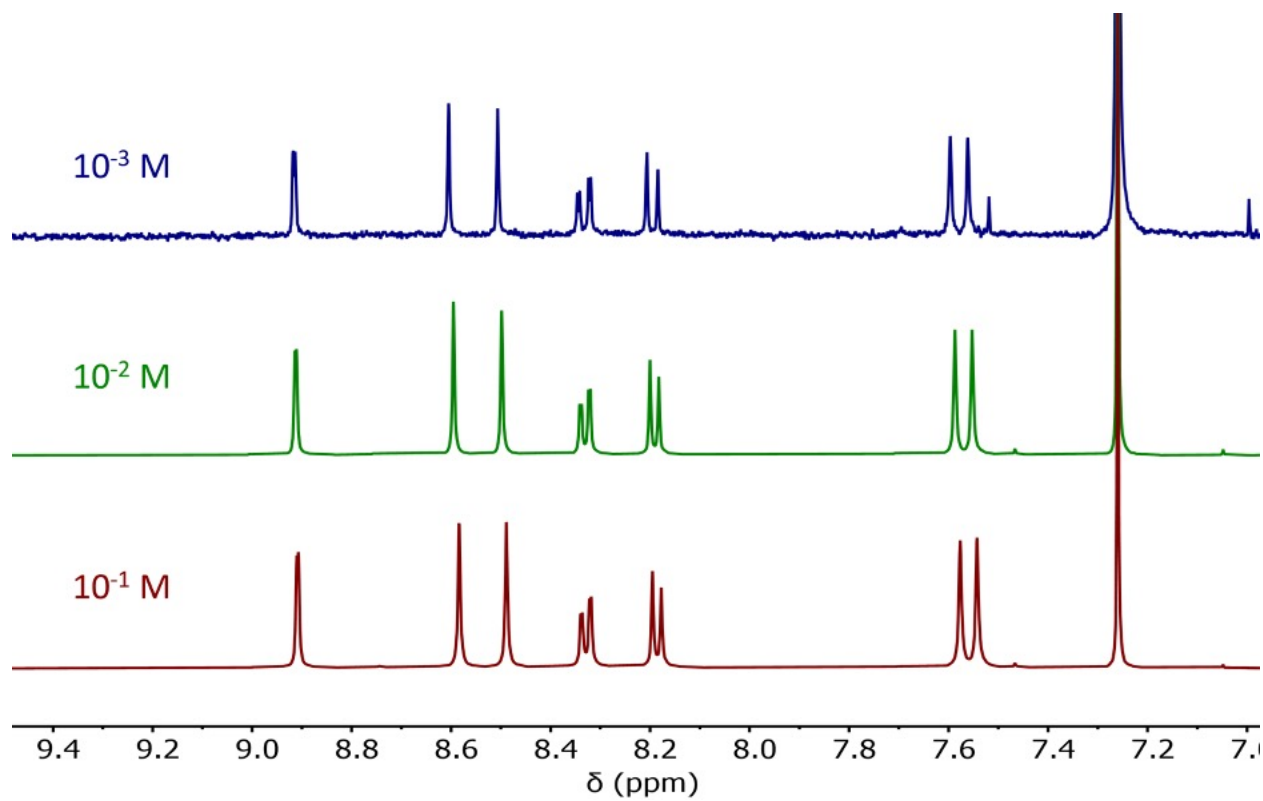


Figure S9. Aromatic region of ^1H NMR of **dDBP(trans)** at $10^{-1} - 10^{-3}$ M.

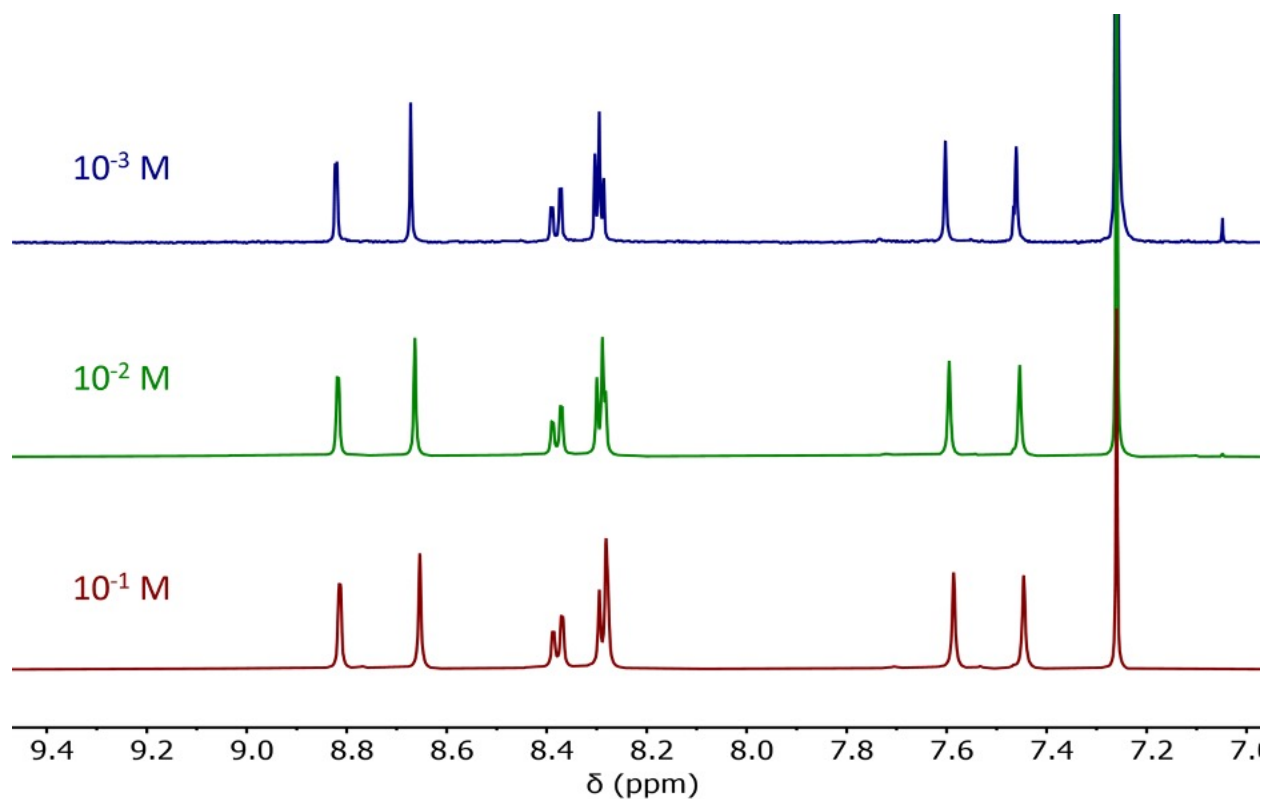


Figure S10. Aromatic region of ^1H NMR of **dDBP(cis)** at $10^{-1} - 10^{-3}$ M.

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.

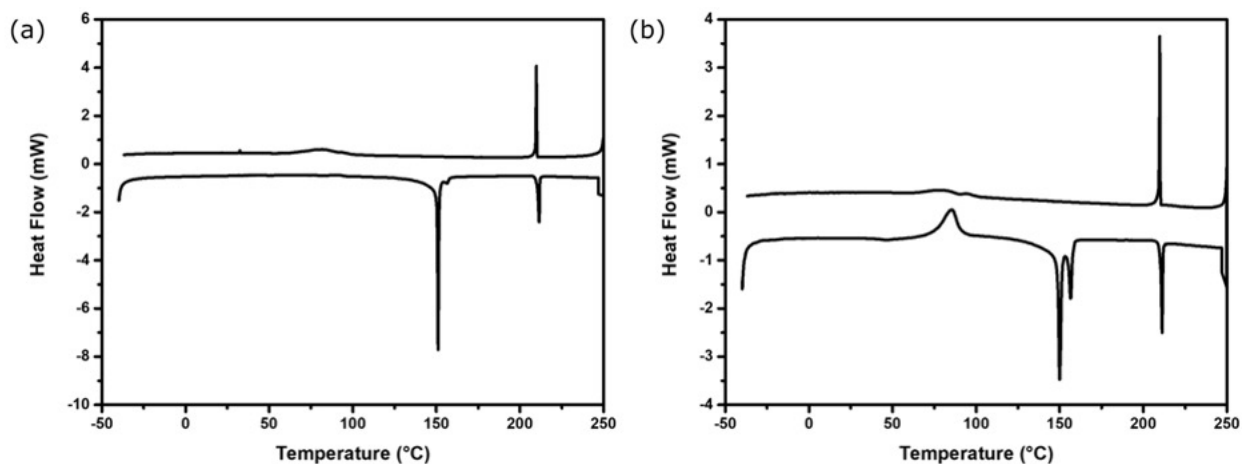


Figure S11. DSC thermograms of **mDBP(trans)** for the (a) first and (b) second heating/cooling cycles.

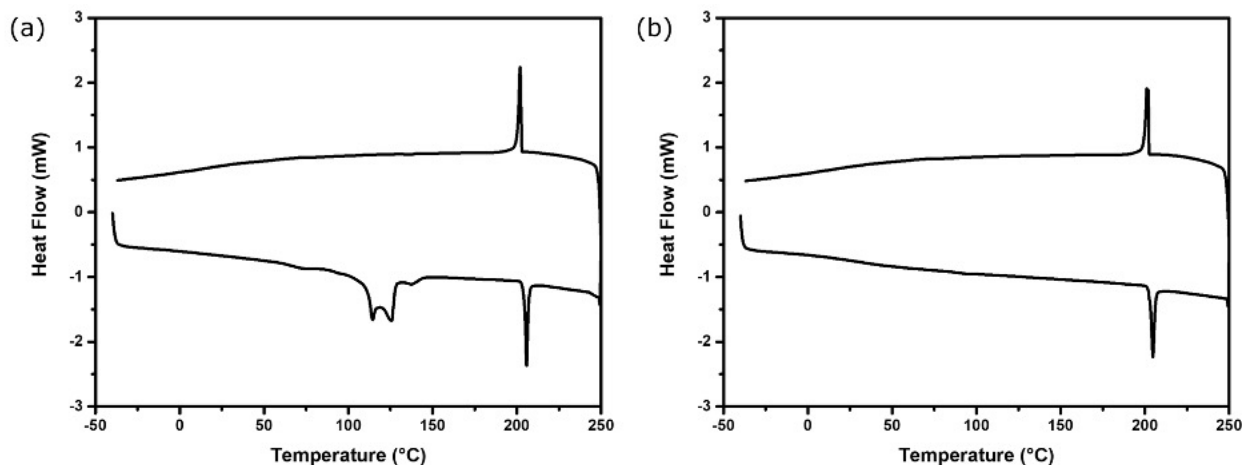


Figure S12. DSC thermograms of **mDBP(cis)** for the (a) first and (b) second heating/cooling cycles.

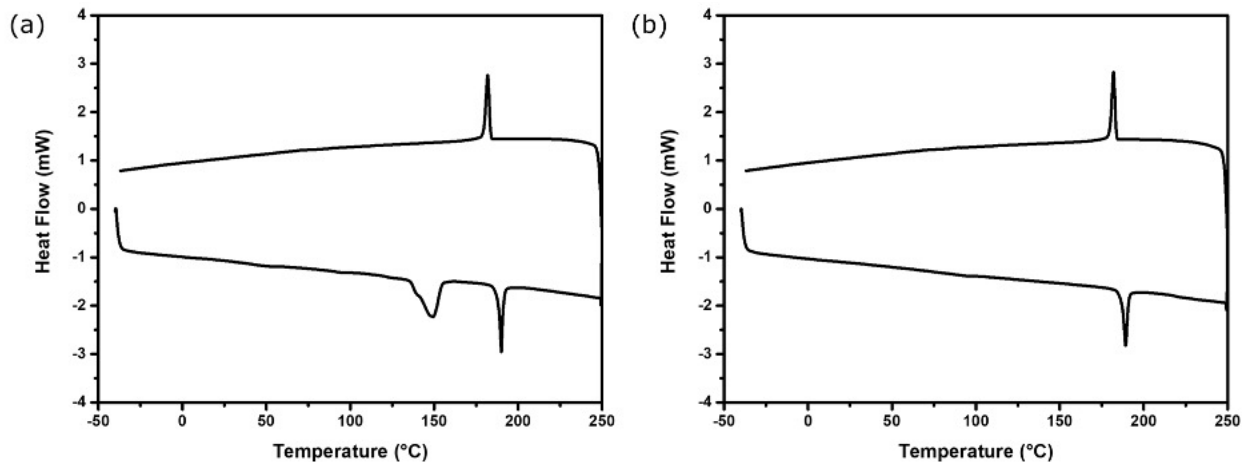


Figure S13. DSC thermograms of **dDBP(trans)** for the (a) first and (b) second heating/cooling cycles.

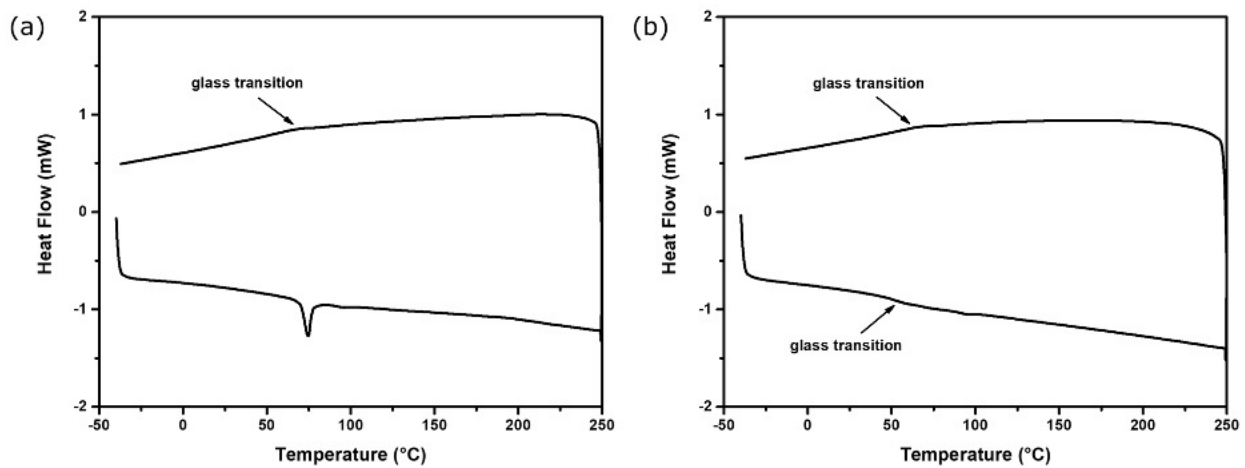


Figure S14. DSC thermograms of **dDBP(cis)** for the (a) first and (b) second heating/cooling cycles.

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.

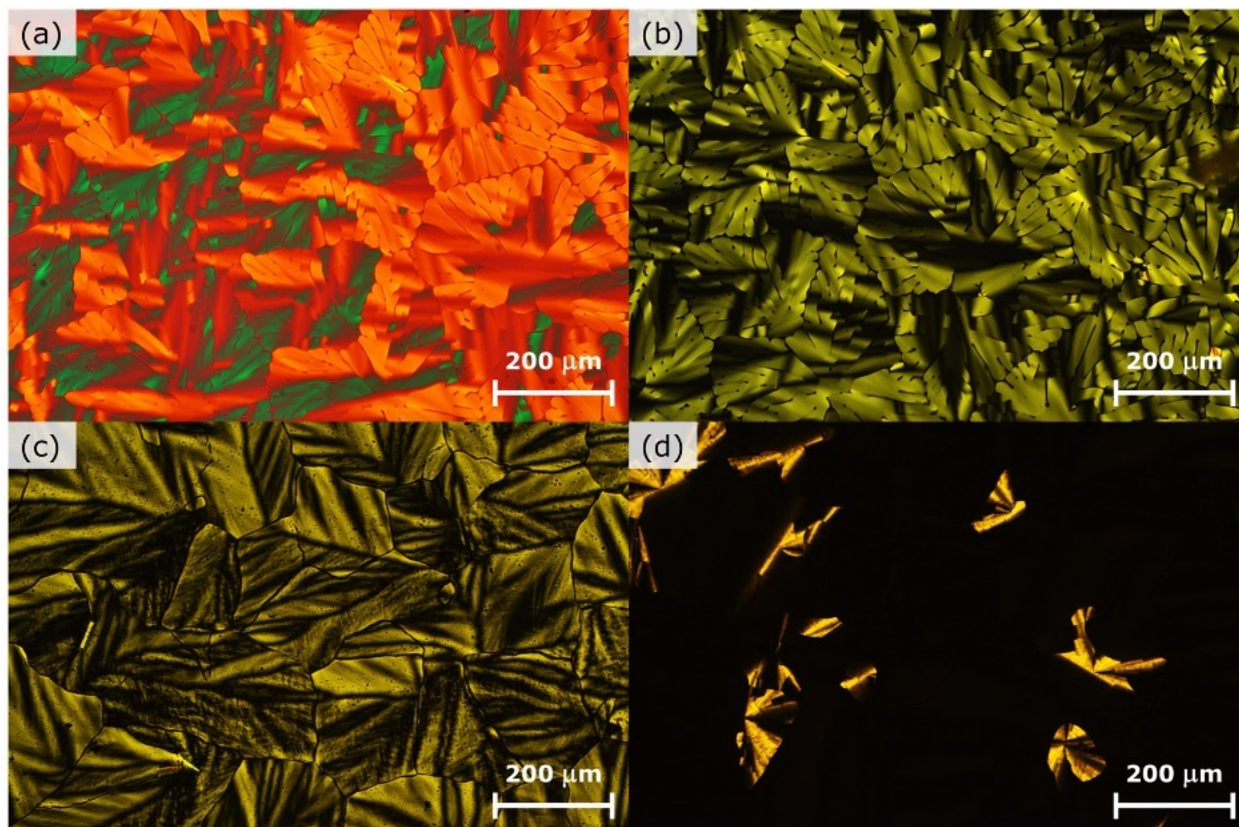


Figure S15. Polarized optical micrographs of **mDBP(trans)** showing dendritic textures with sixfold symmetry at (a-b) 209 °C and (c) room temperature. Image (d) shows the sample at room temperature after 1 year. Image (a) was taken with a 530 nm quarter wavelength retardation plate. Images (b) and (c) were taken in the same plane of view.

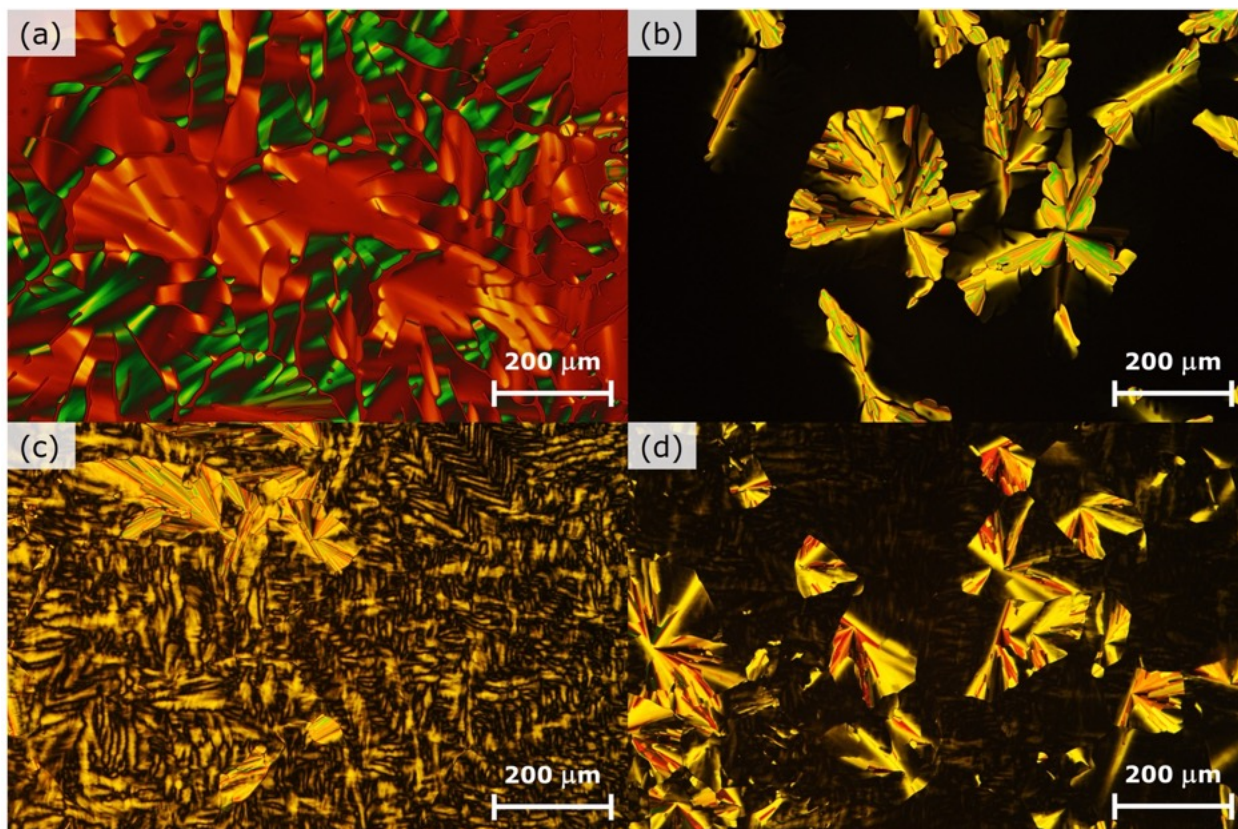


Figure S16. Polarized optical micrographs of **mDBP(cis)** showing dendritic textures with sixfold symmetry at (a-b) 203 °C and (c) room temperature. Image (d) shows the sample at room temperature after 1 year. Image (a) was taken with a 530 nm quarter wavelength retardation plate.

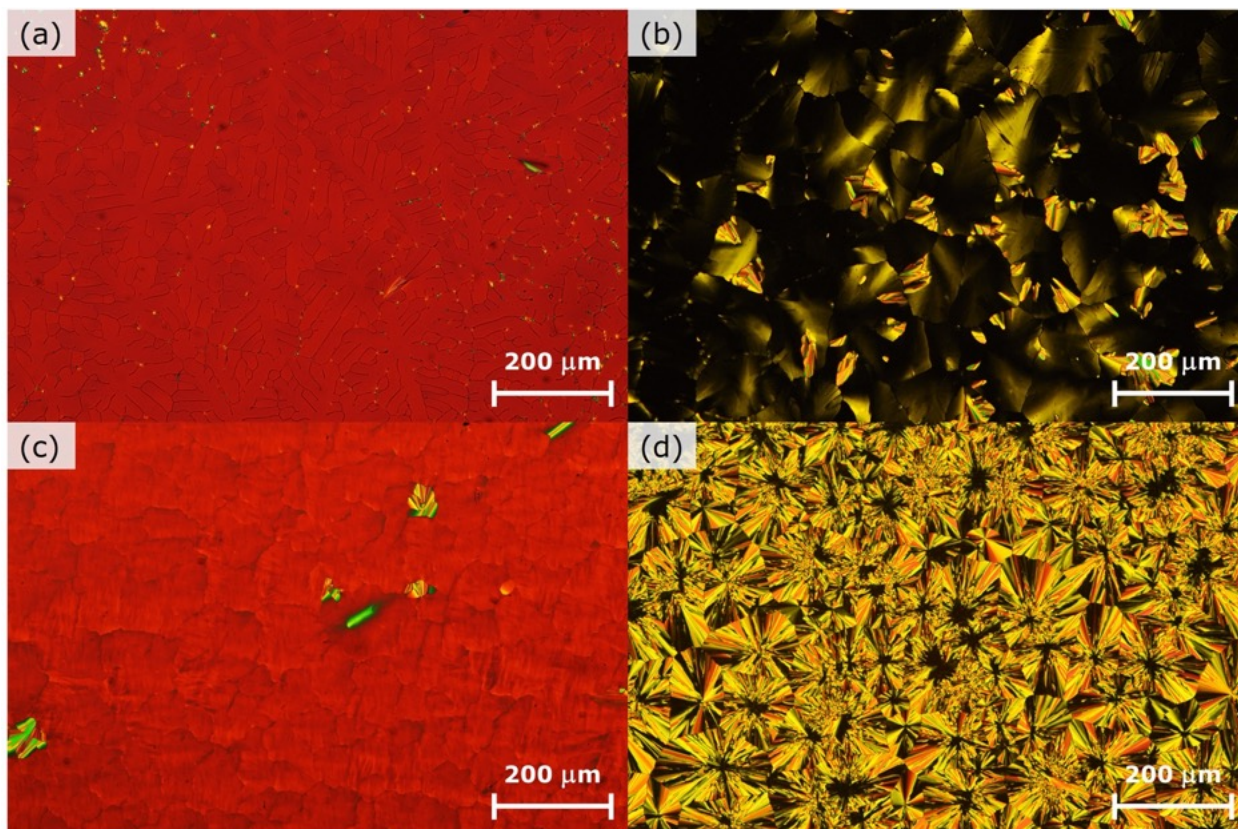


Figure S17. Polarized optical micrographs of **dDBP(trans)** showing dendritic textures with sixfold symmetry at (a-b) 188 °C and (c) room temperature. Image (d) shows the sample at room temperature after 3 years. Images (a) and (c) were taken with a 530 nm quarter wavelength retardation plate.

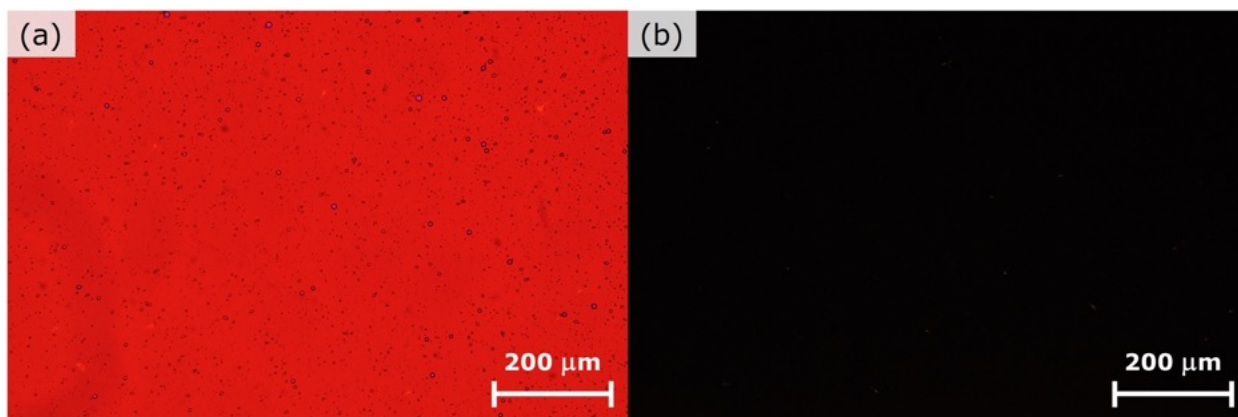


Figure S18. Polarized optical micrographs of **dDBP(cis)** showing the isotropic nature of the material at room temperature (a) with and (b) without a 530 nm quarter wavelength retardation plate.

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

Wide-angle X-ray scattering (WAXS) experiments were obtained on a SAXSLAB Ganesha 300XL Small Angle X-ray Scattering (SAXS) system. All samples were loaded into thin-walled Quartz capillary tubes with a 1.5 mm outer diameter (Charles Supper Company). All measurements were performed using on a Linkam T95-PE heating stage. Figure S19 shows the WAXS spectra of a blank sample and **dDBP(trans)** in the isotropic liquid phase for reference.

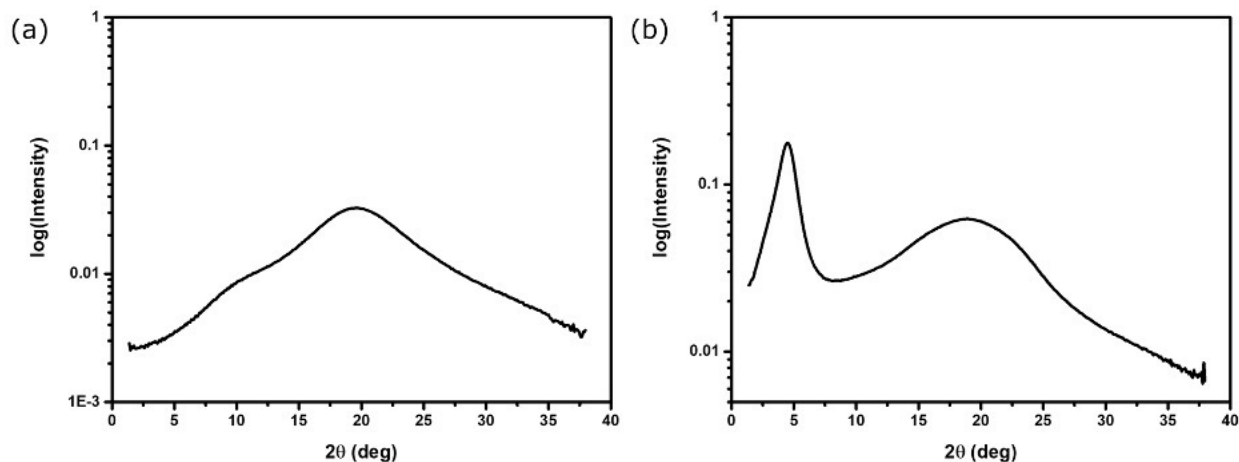


Figure S19. X-ray diffractograms of (a) a blank capillary tube and (b) **dDBP(trans)** in the isotropic liquid phase at 250 °C.

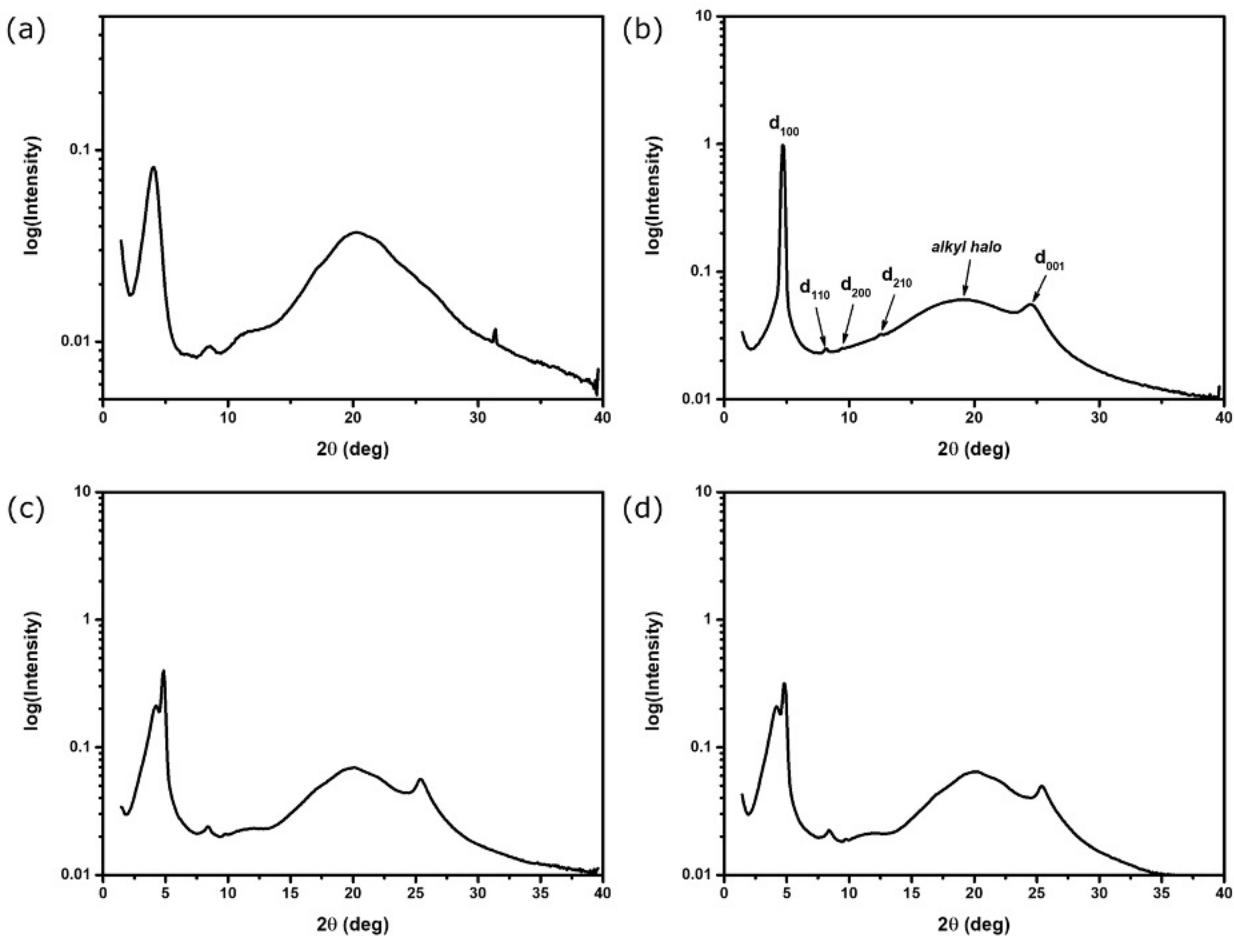


Figure S20. X-ray diffractograms of **mDBP(trans)** at (a) room temperature prior to heating, (b) 200 °C, (c) room temperature after cooling, and (d) room temperature after being left at ambient conditions for 3 days.

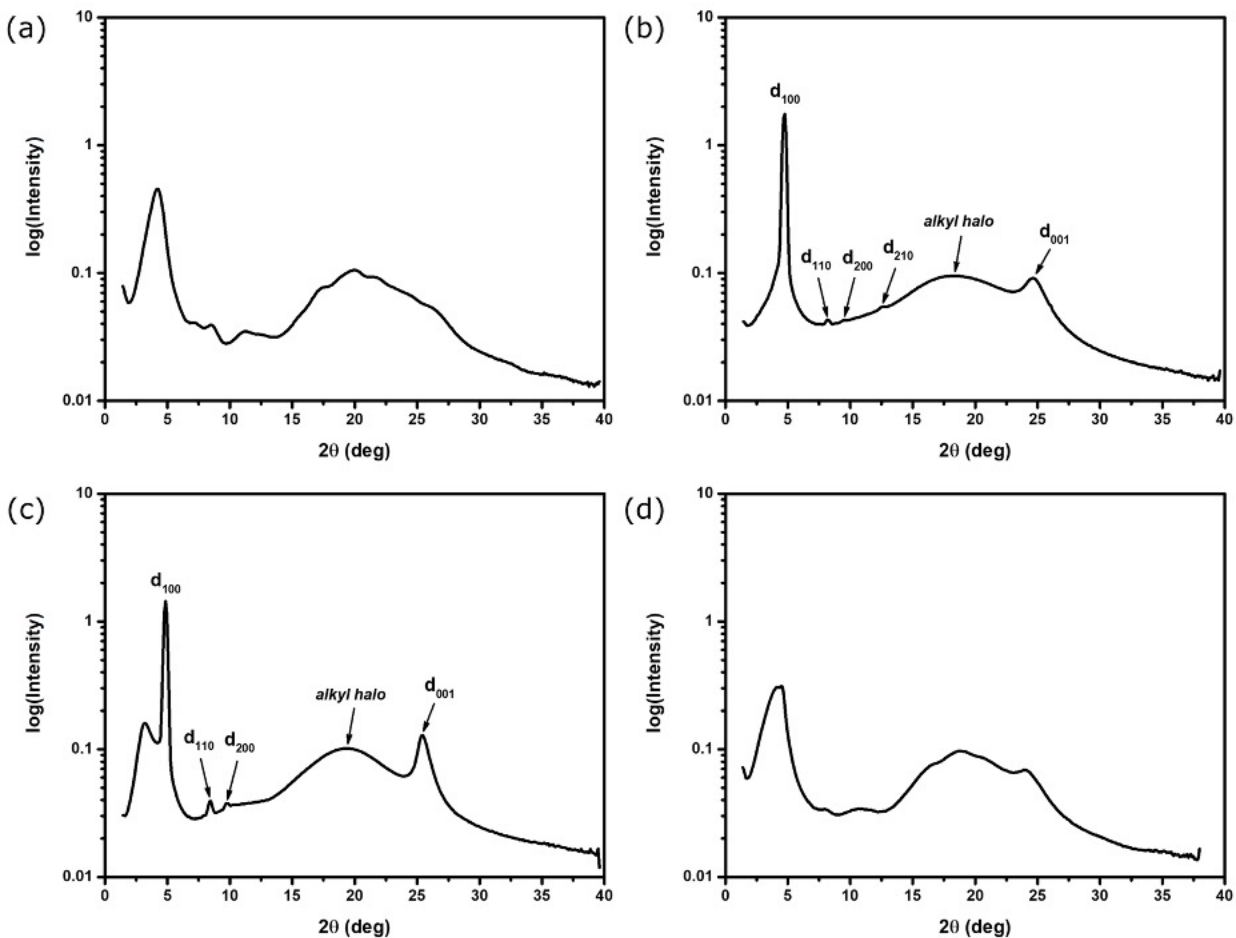


Figure S21. X-ray diffractograms of **mDBP(cis)** at (a) room temperature prior to heating, (b) 190 °C, (c) room temperature after cooling, and (d) room temperature after being left at ambient conditions for 1 year.

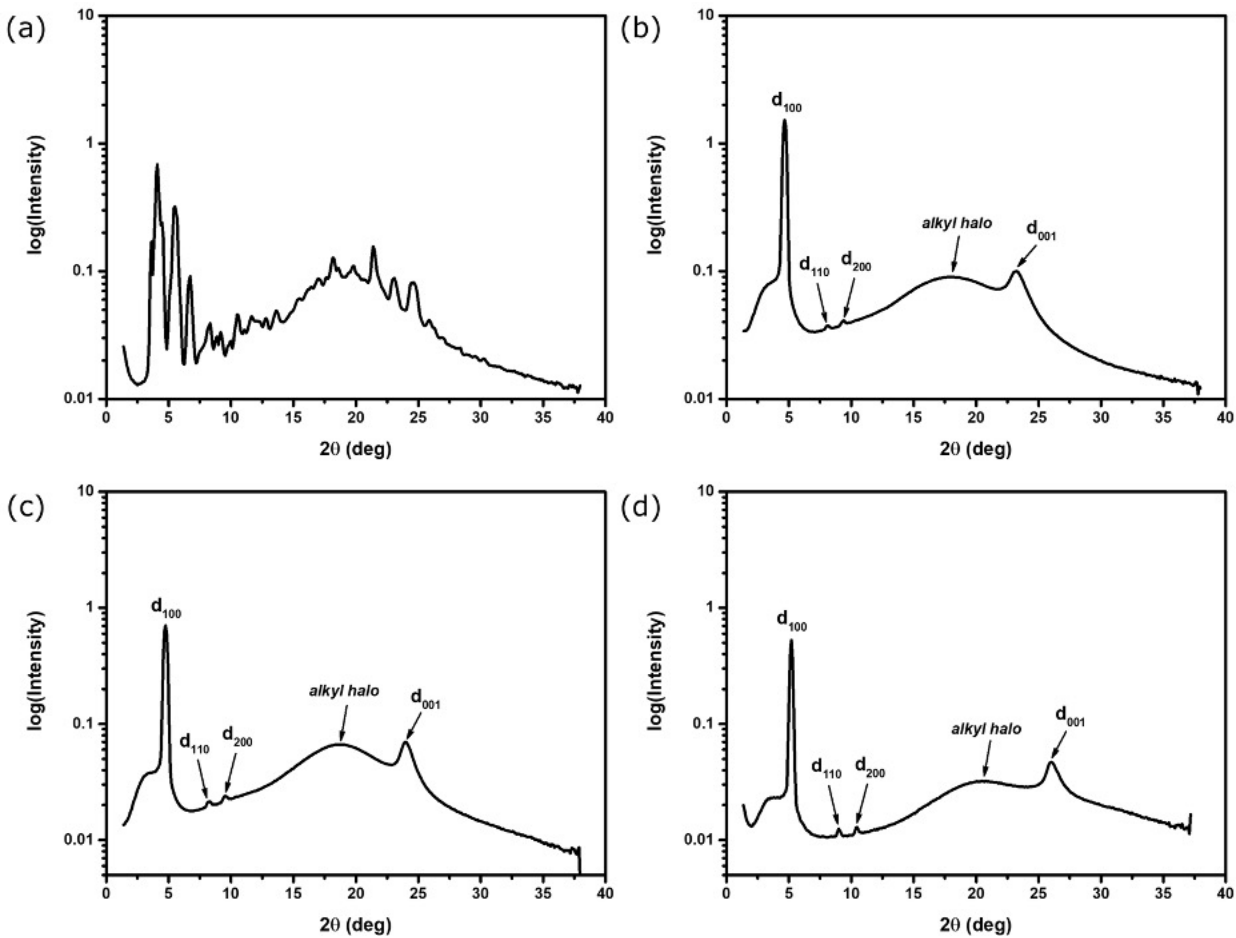


Figure S22. X-ray diffractograms of **dDBP(trans)** at (a) room temperature prior to heating, (b) 180 °C, (c) room temperature after cooling, and (d) room temperature after being left at ambient conditions for over 4 years.

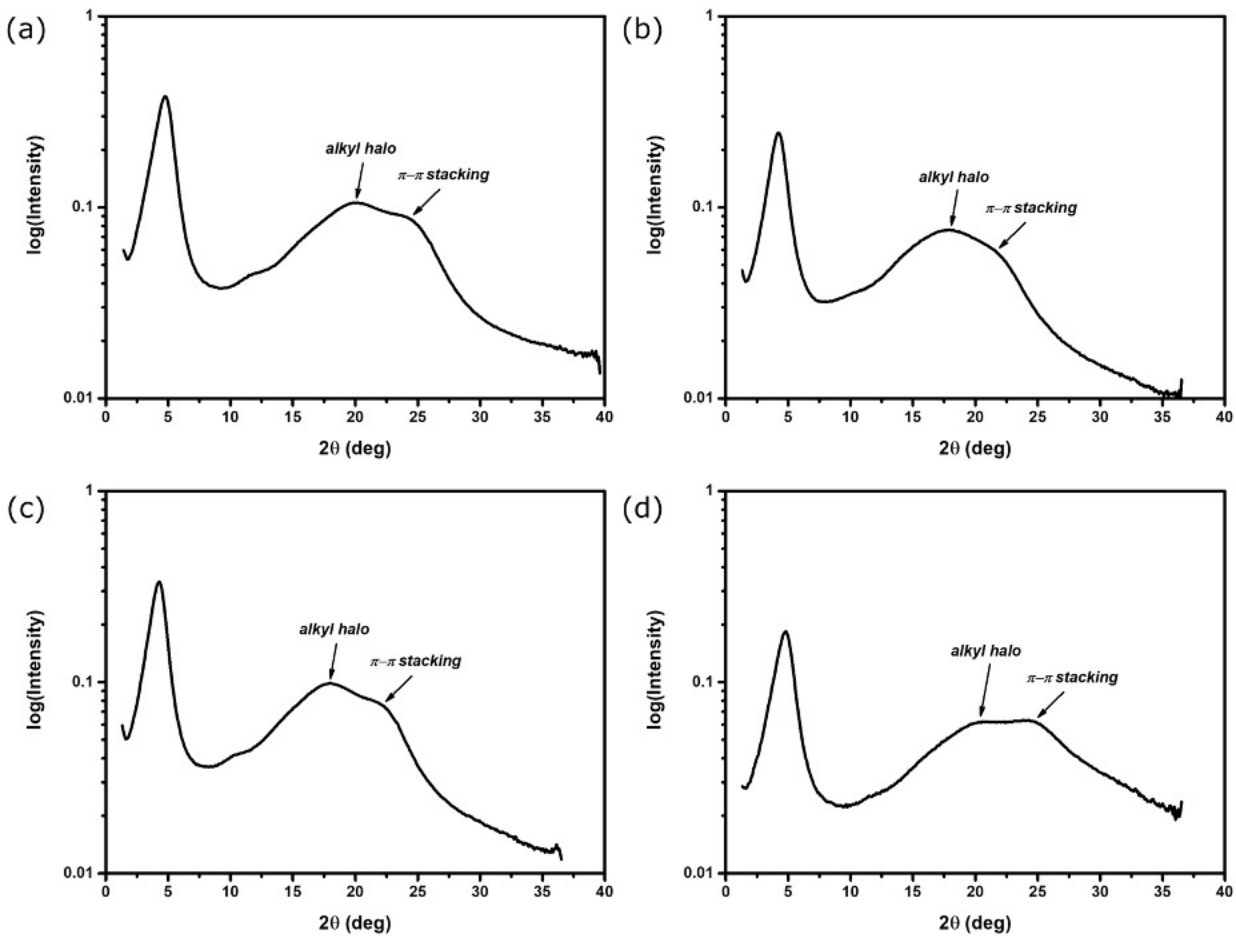


Figure S23. X-ray diffractograms of **dDBP(cis)** at (a) room temperature prior to heating, (b) 150 °C, (c) room temperature, and (d) room temperature after being left at ambient conditions for over 4 years.

Table S1. X-ray diffraction data of the 1,2-cyclohexyl DBP mono- and diesters.

Compound	T (°C)	d-spacings (Å)	Miller Index (hkl)	Phase (lattice constant)	LC Glass Stability
mDBP(trans)	200	19.0	(100)	Col _h (<i>a</i> = 21.9 Å)	< 1 day by DSC and XRD
		10.9	(110)		
		9.3	(200)		
		7.1	(210)		
		4.6	alkyl halo		
		3.6	π-π stacking		
mDBP(cis)	190	18.6	(100)	Col _h (<i>a</i> = 21.4 Å)	< 1 year by XRD
		10.8	(110)		
		9.2	(200)		
		7.0	(210)		
		4.8	alkyl halo		
		3.6	π-π stacking		
dDBP(trans)	180	18.9	(100)	Col _h (<i>a</i> = 21.9 Å)	> 4 years by DSC, POM, and XRD
		10.8	(110)		
		9.4	(200)		
		4.9	alkyl halo		
		3.8	π-π stacking		
		dDBP(cis)	rt		
4.4	alkyl halo				
3.5	π-π stacking				

5. Diffusion Ordered Spectroscopy (DOSY)

Diffusion ordered spectroscopy (DOSY) measurements were obtained on a Bruker AVANCE III digital NMR spectrometer running *TopSpin* version 3.5 with a standard bore magnet operating at 14.1 T (600.13 MHz for ^1H). A Bruker QCI-F 5mm cryoprobe with a Z-gradient coil was used. The sample was exposed to ^1H 90-degree r.f. pulses of 11.6 μs , and a GREAT 1/10 gradient amplifier delivered a maximum gradient current of 10 A, corresponding to a gradient strength of 5.35 G/cmA. The gradient strength was calibrated using distilled water. All samples analyzed were dissolved in D-chloroform and the chemical shift was referenced using the residual solvent signal (set to 7.26 ppm). A flow of heated air was used during all NMR experiments to maintain a temperature of 300 K. The ^1H longitudinal relaxation times (T_1) for the nuclei of interest were estimated using 1-dimensional inversion recovery experiments.

DOSY experiments were performed using a pulse sequence incorporating a bipolar gradient pair with spoiler gradients and longitudinal eddy current delays were used. A recycle delay (D1) of 5 s ($> 5 \times T_1$) was used and 16 scans were accumulated to provide sufficient signal to noise. Initially, two 1-dimensional DOSY scans were carried out on each sample to determine the optimal settings for the diffusion gradient length (δ) and the diffusion time (Δ) using the standard Bruker pulse sequence `ledbpgp2s1d` and gradient strengths (GPZ6) of 2% and 95%, respectively. The 95% gradients should have a signal strength of approximately 5% of the signal intensity observed for a gradient strength of 2%. The delay for longitudinal eddy current dissipation (D21) was set to 5 ms. Typically, Δ (D20) was set to 100 ms and δ was 1000-1200 μs ($2 \times P30$) to sample data over the entire decay curve and ensure reliable estimates of the diffusion coefficients (D). The spectral width was set to 5000 Hz (12.5 ppm), the transmitter offset was set to 5 ppm, shaped file `SMSQ10.100` were used for all gradients, 1 ms spoiler gradients were set to -17.13% (GPZ7) and -13.17% (GPZ8) of maximum power and the gradient recovery delay (D16) was set to 200 μs .

After setting up the DOSY measurement parameters, a linear ramp of the gradient strengths from 2-95% was employed using the `au` program “`dosy`” to create the gradient ramp file. A pseudo-2-D array of 16 x 1-D NMR experiments was acquired using the standard Bruker pulse sequence `ledbpgp2s` (total experiment time was 3-4 h). The DOSY data was processed by applying a 1-dimensional Fourier transform in the F2 direction (`xf2`) with a 2 Hz exponential apodization, phased and baseline corrected (`abs2`). The `au` program “`setdiffparm`” was run to extract diffusion sequence parameters and store parameters for DOSY processing. To determine the diffusion coefficients, D , for each sample, integrated peak areas for the four phenanthrene protons in the aromatic region were fit to the gradient strength. Fitting was done using the T_1/T_1 analysis routines in *TopSpin* on peak intensity against gradient strength, which is fit to equation S1 to determine the values of D in units of m^2/s . The D was calculated from each of the four phenanthrene proton peaks, with the reported D representing an average of each of these values (see Table S2).

$$I = I_0 e^{-D\gamma^2 g^2 \delta^2 (\Delta - \frac{\delta}{3} \frac{\tau}{2})} \quad (\text{S1})$$

Table S2. DOSY data obtained for all six dimers discussed in the manuscript.

Compound	Diffusion Coefficient, D (* $10^{-9} \text{ m}^2\text{s}^{-1}$)	Standard Deviation (* $10^{-9} \text{ m}^2\text{s}^{-1}$)
dDBP(trans)	2.06	0.01
dDBP(cis)	1.89	0.02
dDBP(2R,3R)	2.00	0.02
dDBP(meso)	2.00	0.02
dDBP(cat)	3.81	0.02
dDBP(hyd)	1.69	0.01

6. Conformational Dynamics Data

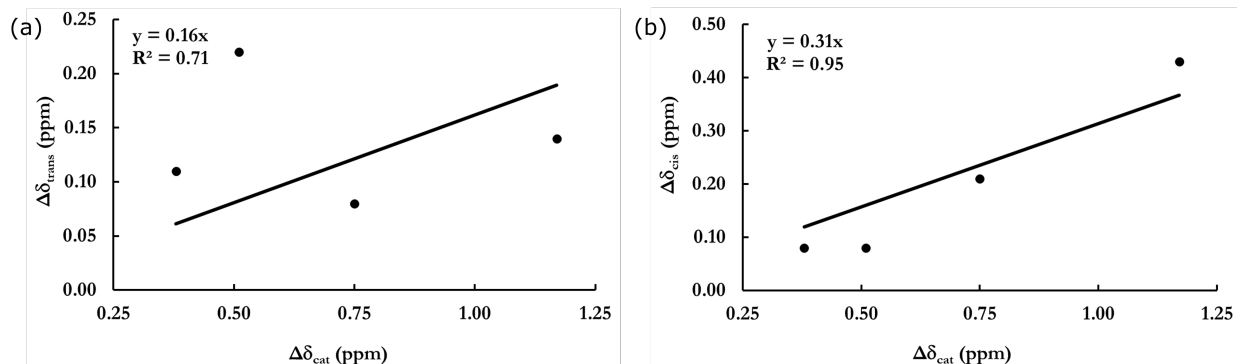


Figure S24. Experimental $\Delta\delta$ values of (a) **dDBP(trans)** and (b) **dDBP(cis)** against **dDBP(cat)**.

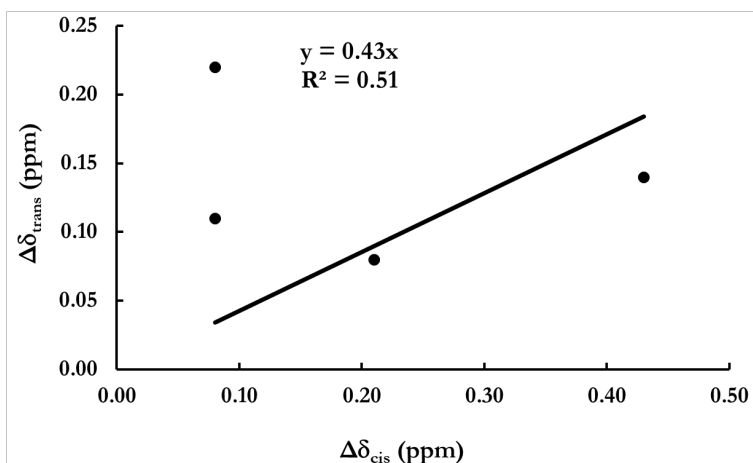


Figure S25. Experimental $\Delta\delta$ values of **dDBP(trans)** against **dDBP(cis)**.

7. Modelling Schematics

Shown below are the lowest energy conformers of **dDBP(trans)** and **dDBP(cis)** as well as side-by-side comparisons of the folded and unfolded conformers of **dDBP(trans)** and **dDBP(2R,3R)** and of **dDBP(cis)** and **dDBP(meso)**. In addition, the optimized structure of **dDBP(cat)** and **dDBP(hyd)** are shown.

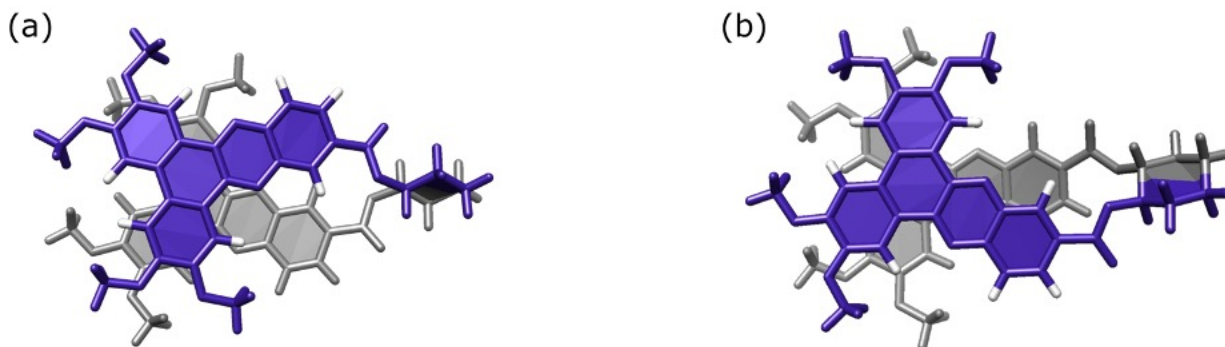


Figure S26. (a) Lowest energy folded conformer and (b) the folded conformer that best fit the ¹H NMR data for **dDBP(trans)**.

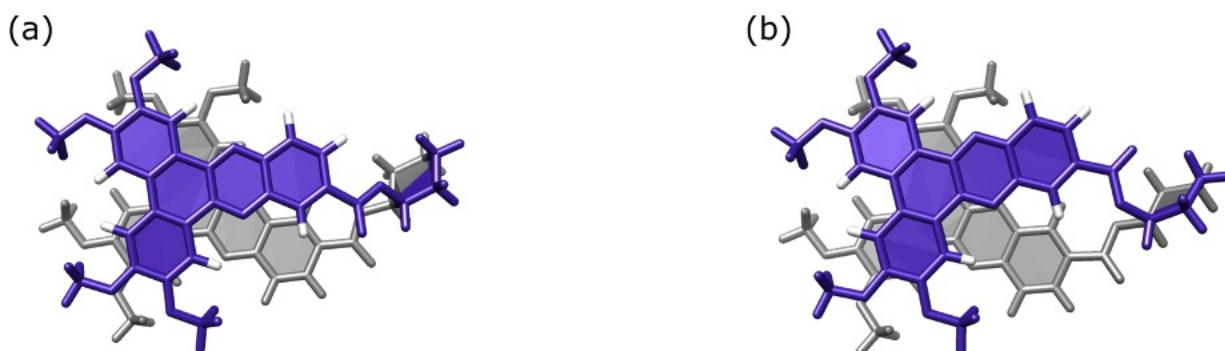


Figure S27. (a) Lowest energy folded conformer and (b) the folded conformer that best fit the ¹H NMR data for **dDBP(cis)**.

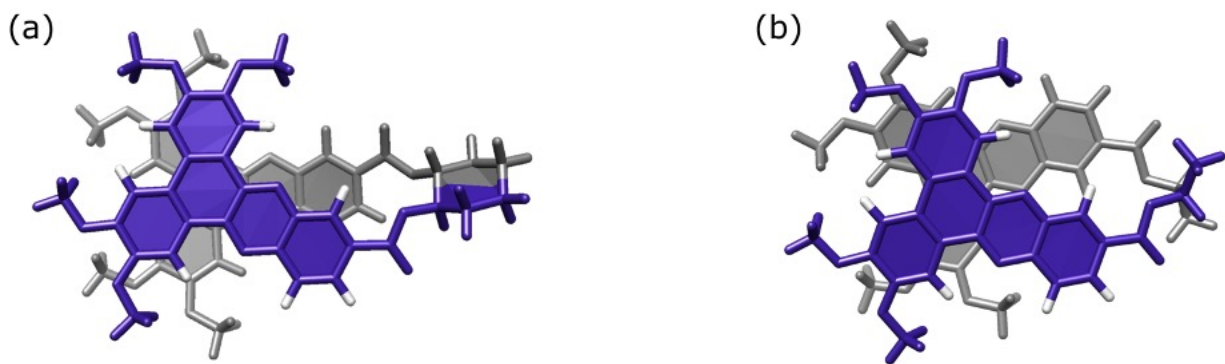


Figure S28. Folded conformers that best fit the ¹H NMR data for (a) **dDBP(trans)** and (b) **dDBP(2R,3R)**.

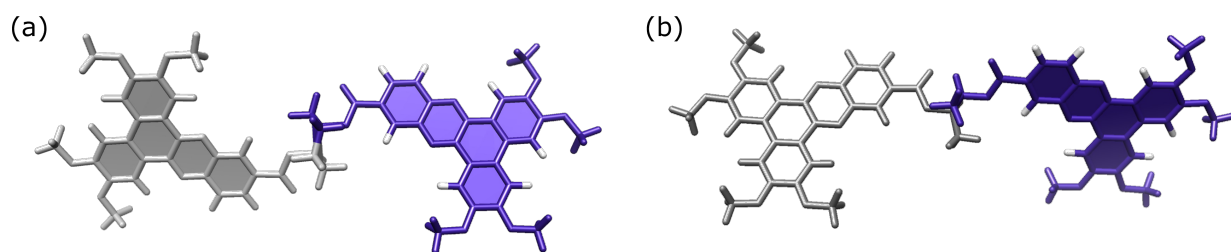


Figure S29. Lowest energy unfolded conformers of (a) **dDBP(trans)** and (b) **dDBP(2R,3R)**.

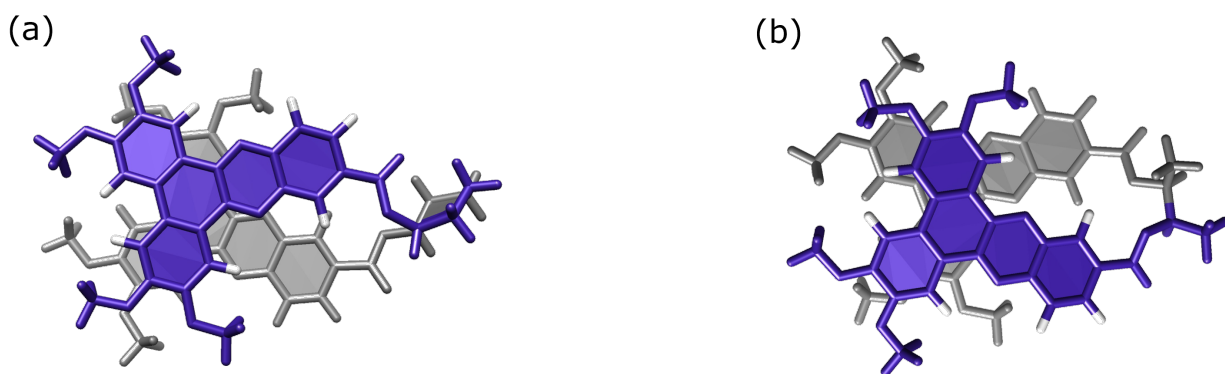


Figure S30. Folded conformers that best fit the ^1H NMR data for (a) **dDBP(cis)** and (b) **dDBP(meso)**.

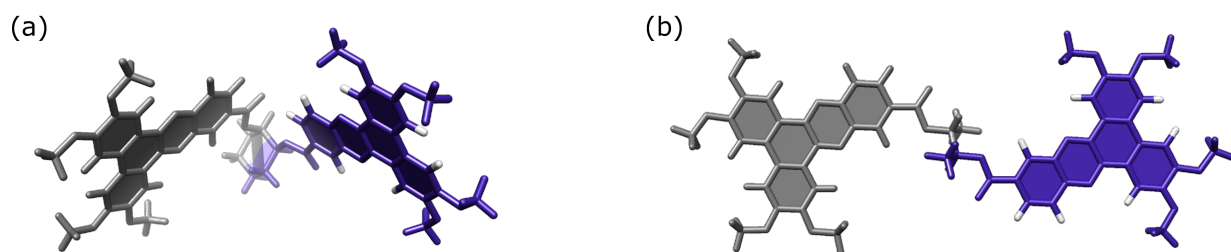


Figure S31. Lowest energy unfolded conformers of (a) **dDBP(cis)** and (b) **dDBP(meso)**.

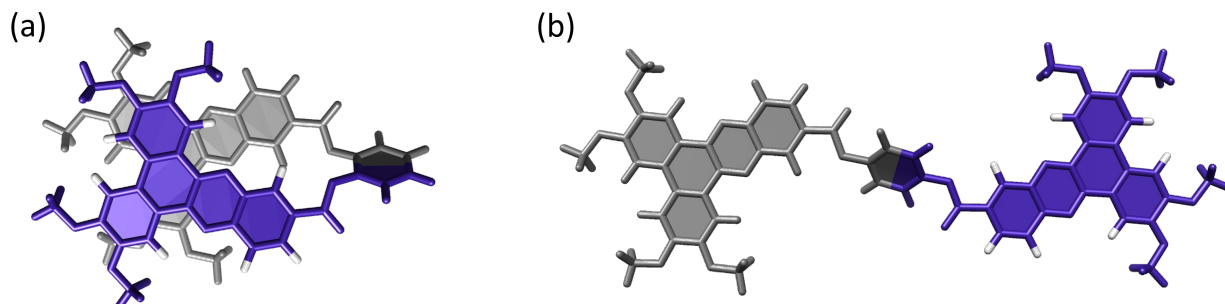


Figure S32. Optimized structures of (a) **dDBP(cat)** and (b) **dDBP(hyd)**.

8. Modelling Details

I. Optimization Methods

General Calculation Details

All calculations were carried out using Gaussian 09¹ 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 this thesis 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)² calculations using the Becke three parameter Lee-Yang-Parr (B3LYP) method^{3,4} at the 6-31G(d) level.^{5,6} 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 of a given compound depends on the complexity and flexibility of the molecule (see Monomers and Dimers sections below). Note this information describes modelling for the 1,2-cyclohexyl diastereomeric derivatives only. Please see supporting information from our previous work: C. O. Zellman and V. E. Williams, *J. Org. Chem.*, 2021, **86**, 15076-15084 (<https://pubs.acs.org/doi/10.1021/acs.joc.1c01626>) for modelling details on the 2,3-butyl, catechol, and hydroquinone systems.⁷

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(MeE)** (Figure S33(a)) for example, shows the two main conformations the ester group can adopt: the carbonyl can be syn (Figure S33(b)) or anti (Figure S33(c)) to H_a on the DBP core. The two conformations of **DBP(MeE)** are then optimized by DFT calculations using the method described in the “General Calculation Details” above. In addition, a dispersion correction was applied: the Grimme D3 dispersion correction (B3LYP-D3 functional).^{8,9} This was not necessary for the monoesters, but it did prove vital when optimizing conformations of the dimers (see later); hence, the B3LYP-D3 functional was used to maintain consistency between the calculations of mono- and diesters. The conformations of all monomers are summarized in the Results section (section III).

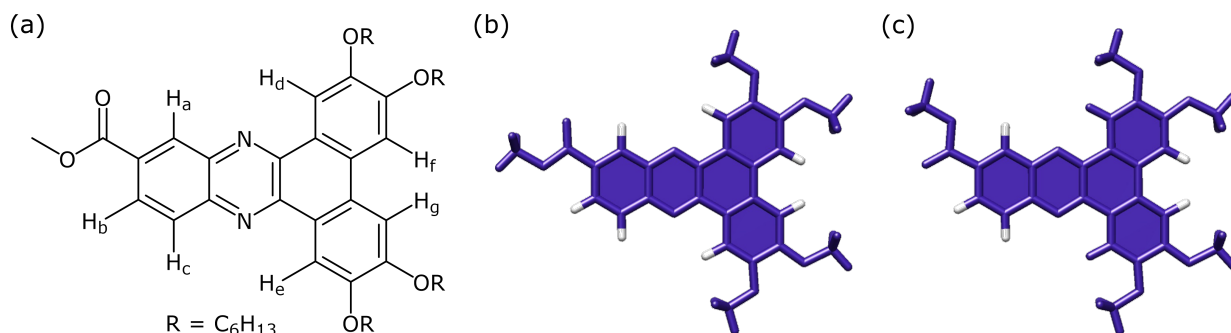


Figure S33. (a) Schematic of **DBP(MeE)**, outlining the seven protons on the DBP ring. Note protons *d* and *e* cannot be distinguished by 2D NMR, and likewise for protons *f* and *g*. Assignment of protons *d* and *e* was devised by comparing the calculated chemical shifts to the experimental chemical shifts, and likewise for protons *f* and *g*. The two optimized conformers of **DBP(MeE)** 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 two diesters, there are various conformations that can be adopted, including both folded and unfolded geometries. The number of conformers for a given dimer was determined by considering a few geometrical factors: (i) the number of non-degenerate chair conformations (we assume the linker predominantly adopts the chair conformation); (ii) the configuration of the two esters with respect to the linker; (iii) 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.

As an example, Figure S34 outlines all the possible conformations of the (1R,2R)-*trans*-1,2-cyclohexyl DBP diester (**dDBP(trans)**). For **dDBP(trans)**, there are (i) two possible chair configurations: the diequatorial (**dEq**) or diaxial (**dAx**) conformers. There are (ii) three possible configurations between the two esters and the linker: both carbonyls of the ester are syn to the methine hydrogen (**+1**), one carbonyl is syn and one is anti to the methine hydrogen (**0**), or both carbonyls are anti to the methine hydrogen (**-1**) of the cyclohexyl ring. Finally, there are (iii) 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.

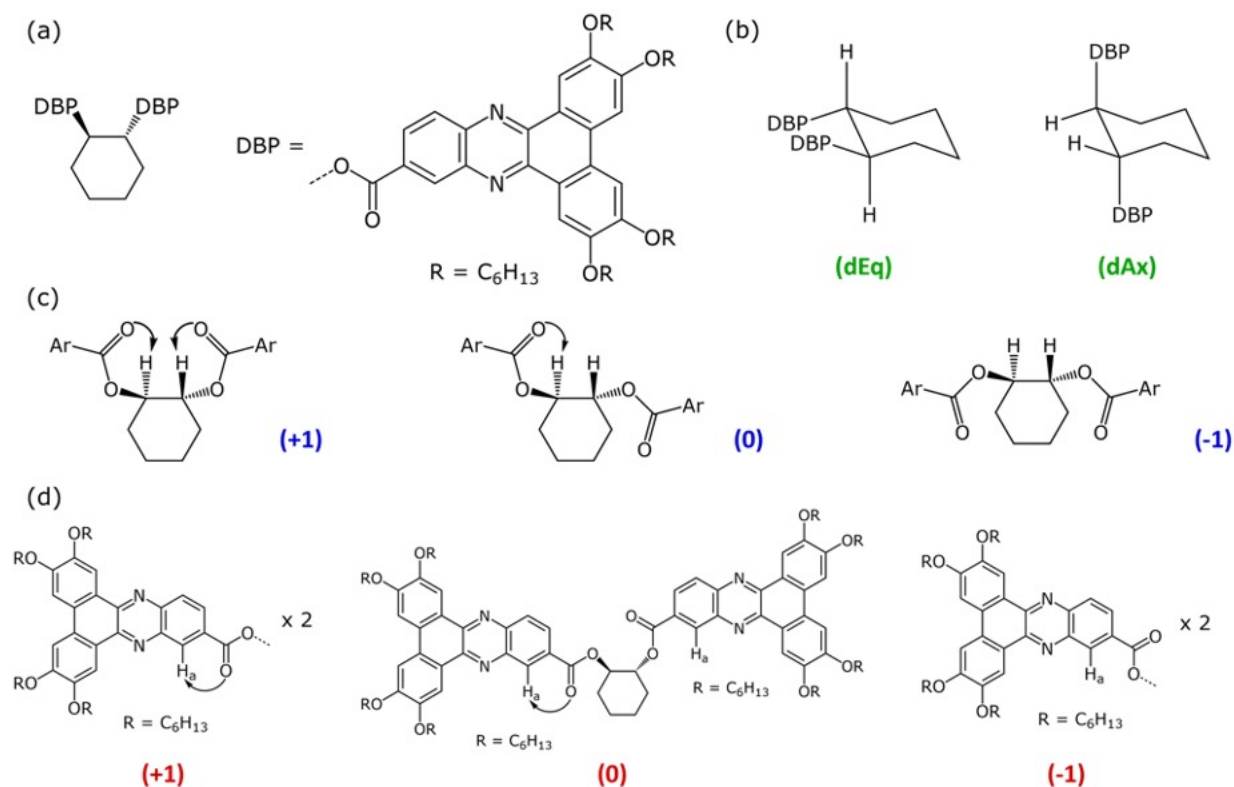


Figure S34. Schematics of (a) the chemical structure of **dDBP(trans)**, (b) the two possible chair conformations of **dDBP(trans)**, (c) the three possible conformations of the diester with respect to the linker (Ar = DBP core), and (d) the three conformations between the diester and the DBP cores.

As outlined in Figure S34, each type of conformation is labelled to help keep track of all the possible conformations. For **dDBP(trans)**, summing all configurations yields a total of $2 \times 3 \times 3 = 18$ conformations; however, there are 20 conceivable conformations for **dDBP(trans)** using the method of analysis outlined in Figure S34. The extra two conformations arise because for the **dEq** and **dAx** configurations, when (ii) is 0 and (iii) is 0, there are two possible scenarios: the carbonyl that is syn to the methine hydrogen of the cyclohexyl 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 chair configurations, and therefore there are a total of 20 possible conformations for **dDBP(trans)**.

The *cis*-1,2-cyclohexyl dimer, **dDBP(cis)**, was studied in a similar fashion. The total number of conformers, along with the relative energies for both dimers are summarized in the Results section (section III).

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 in Gaussian 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).¹⁰ The structures were then optimized again with DFT² calculations using the B3LYP method^{3,4} at the 6-31G(d) level^{5,6} with an added Grimme D3 dispersion correction (B3LYP-D3 functional).^{8,9} The dispersion correction was especially important for folded conformations because non-corrected DFT calculations often view π - π interactions as repulsive.¹¹

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 a molecular mechanics pre-optimization were significantly more computationally expensive.

II. NMR Calculations

General Calculation Details

The ¹H NMR of each folded conformation was calculated from the optimized geometries. The standard Gauge-Independent Atomic Orbital (GIAO) approach¹² was used for the ¹H NMR calculations at the DFT level (B3LYP-D3, 6-31G(d)) used to optimize the structures. The GIAO approach has proven useful in calculating the magnetic shielding of protons for a wide variety of molecules.^{13,14} The calculated ¹H NMRs for each conformation was then compared with the experimental ¹H NMR data. The details of these analyses are summarized in the “Monomers” and “Dimers” sections below.

Monomers

For each monoester, the ¹H 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 09.¹ 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 ¹H NMR calculations, the average calculated δ_m values were compared with the experimental δ_m values (Figure S35). All monoesters displayed a fit of $R^2 \geq 0.97$; hence, the NMR calculations do appear to accurately depict the experimental aromatic region of the ¹H NMR.

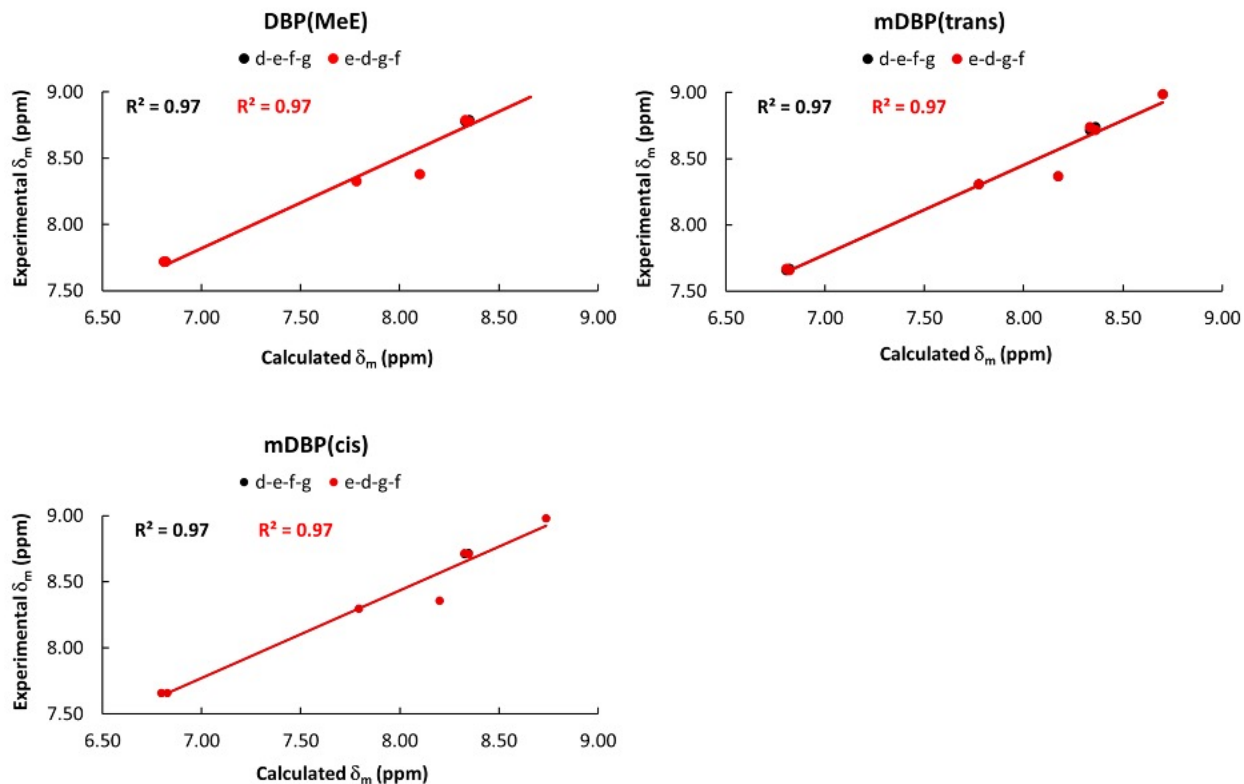


Figure S35. Experimental δ_m versus calculated δ_m plots for **DBP(MeE)**, **mDBP(trans)**, and **mDBP(cis)**. For each graph, two series are plotted: d-e-f-g and e-d-g-f. These two series are plotted separately because, as elucidated in Figure S33, proton pairs *d/e* and *f/g* are indistinguishable 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.

Evidently from Figure S35, the calculated and experimental δ_m values do not change appreciably between the two monomers, suggesting the nature of the ester group does not significantly influence the aromatic chemical shifts. Indeed, the ^1H NMRs are very similar across the monomeric series. To avoid small discrepancies in δ_m values between the monomers, **mDBP(trans)** was used to represent all δ_m values in the analysis. Therefore, all δ_m values reported herein represent the aromatic chemical shifts of **mDBP(trans)**.

Dimers

NMR calculations were performed on all optimized folded conformations for **dDBP(trans)** and **dDBP(cis)**. For each conformer, 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 09.¹ The degree of upfield shift, $\Delta\delta$, for each aromatic proton in a folded conformer with respect to the monomer **mDBP(trans)** was calculated according to equation (S2):

$$\Delta\delta = \delta_m - \delta_d \quad (S2)$$

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 $\Delta\delta$ values were plotted against the calculated $\Delta\delta$ 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 Tables S3 – S5 and Figures S36 – S37. 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(MeE)**, as described in Figure S33.

Table S3. The total number of conformations, energies, relative energies, and number of imaginary frequencies for each conformer of **DBP(MeE)**.

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	(+1/2)	-1564.9269	+0.3	0
2	(-1/2)	-1564.9273	0.0	0

mDBP(trans)

Eight conformations were analyzed for **mDBP(trans)**. The 8 conformations arise from the following geometrical factors: there are two possible configurations for the chair conformation of the cyclohexyl group – the ester is in the equatorial (**Eq**) or axial (**Ax**) position. There are two starting configurations between the ester and the cyclohexyl group – the carbonyl is syn (**+1/2**) or anti (**-1/2**) to the methine hydrogen on the adjacent carbon of the cyclohexyl ring. Finally, 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 S33 for schematic of the DBP core).

Table S4. The total number of conformations, energies, relative energies, and number of imaginary frequencies for each conformer of **mDBP(trans)**.

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	(Eq, +1/2, +1/2)	-1835.5258	+1.9	0
2	(Eq, +1/2, -1/2)	-1835.5262	+1.7	0
3	(Eq, -1/2, +1/2)	-1835.5238	+3.2	0
4	(Eq, -1/2, -1/2)	-1835.5239	+3.1	0
5	(Ax, +1/2, +1/2)	-1835.5284	+0.4	0
6	(Ax, +1/2, -1/2)	-1835.5289	0.0	0
7	(Ax, -1/2, +1/2)	-1835.5166	+7.7	0
8	(Ax, -1/2, -1/2)	-1835.5169	+7.5	0

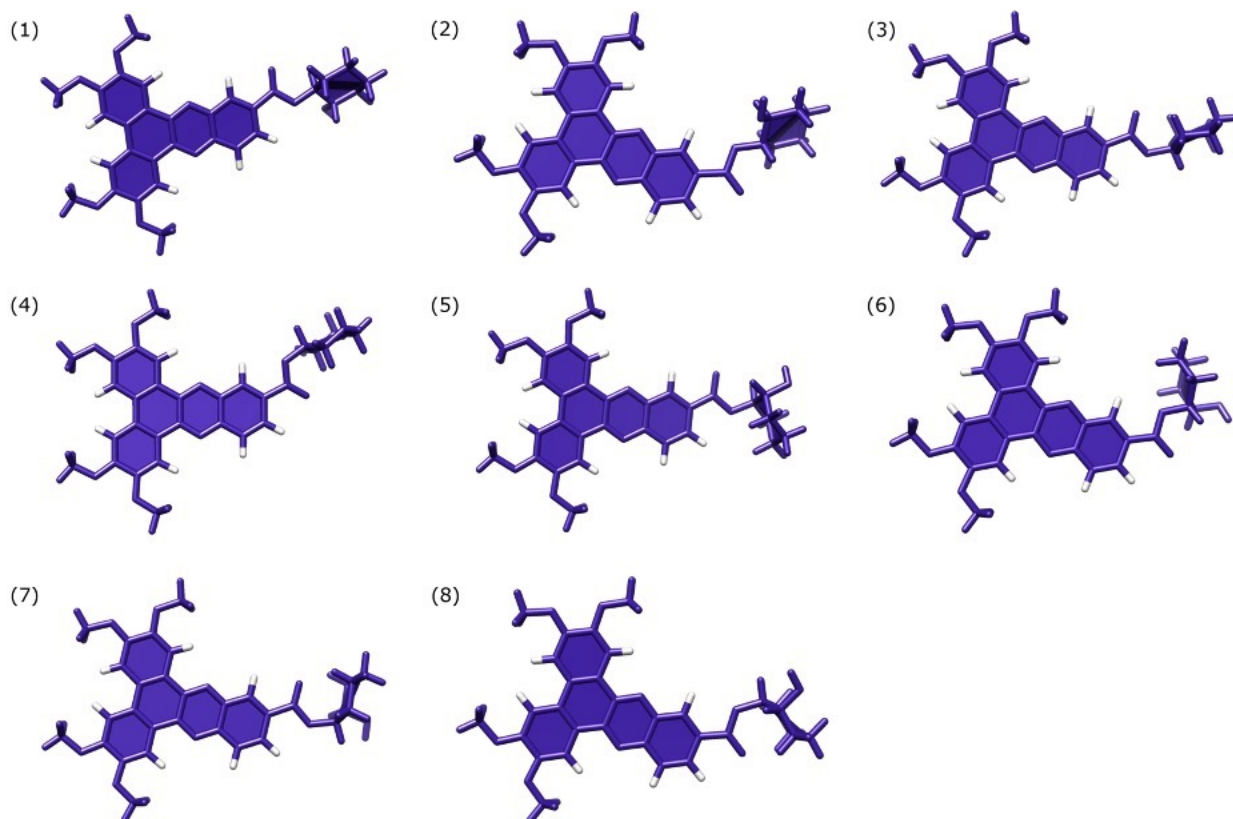


Figure S36. Schematics of all 8 conformations for **mDBP(trans)**. The number displayed in the figure corresponds to the conformation number in Table S4. Hydrogens on the DBP core are shown in light grey.

mDBP(cis)

Eight conformations were analyzed for **mDBP(cis)**. The 8 conformations arise from the following geometrical factors: there are two possible configurations for the chair conformation of the cyclohexyl group – the ester is in the equatorial (**Eq**) or axial (**Ax**) position. There are two starting configurations between the ester and the cyclohexyl group – the carbonyl is syn (**+1/2**) or anti (**-1/2**) to the methine hydrogen on the adjacent carbon of the cyclohexyl ring. Finally, 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 S33 for schematic of the DBP core).

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

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq
1	(Eq, +1/2, +1/2)	-1835.5262	+3.8	0
2	(Eq, +1/2, -1/2)	-1835.5266	+3.5	0
3	(Eq, -1/2, +1/2)	-1835.5174	+9.3	0
4	(Eq, -1/2, -1/2)	-1835.5179	+9.0	0
5	(Ax, +1/2, +1/2)	-1835.5317	+0.3	0
6	(Ax, +1/2, -1/2)	-1835.5322	0.0	0
7	(Ax, -1/2, +1/2)	-1835.5161	+10.1	0
8	(Ax, -1/2, -1/2)	-1835.5165	+9.9	0

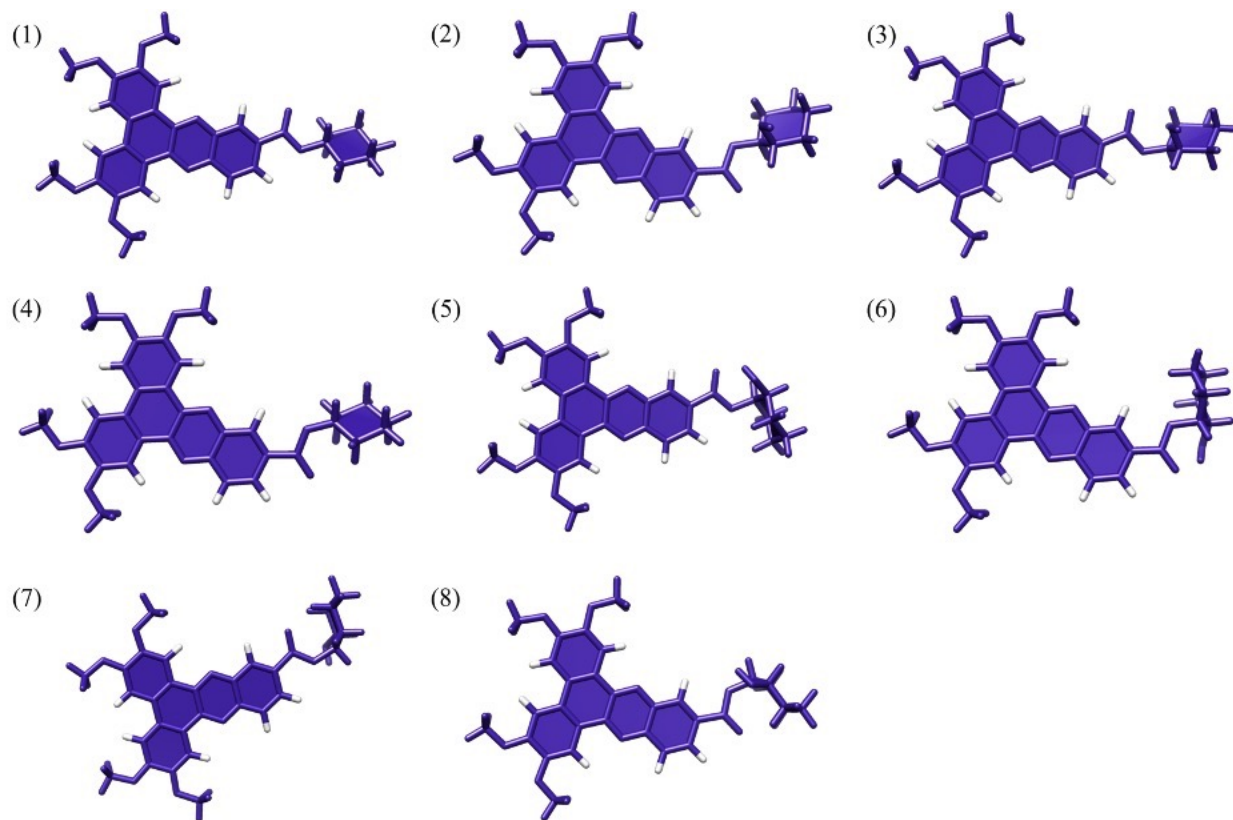


Figure S37. Schematics of all 8 conformations for **mDBP(cis)**. The number displayed in the figure corresponds to the conformation number in Table S5. Hydrogens on the DBP core are shown in light grey.

Dimers

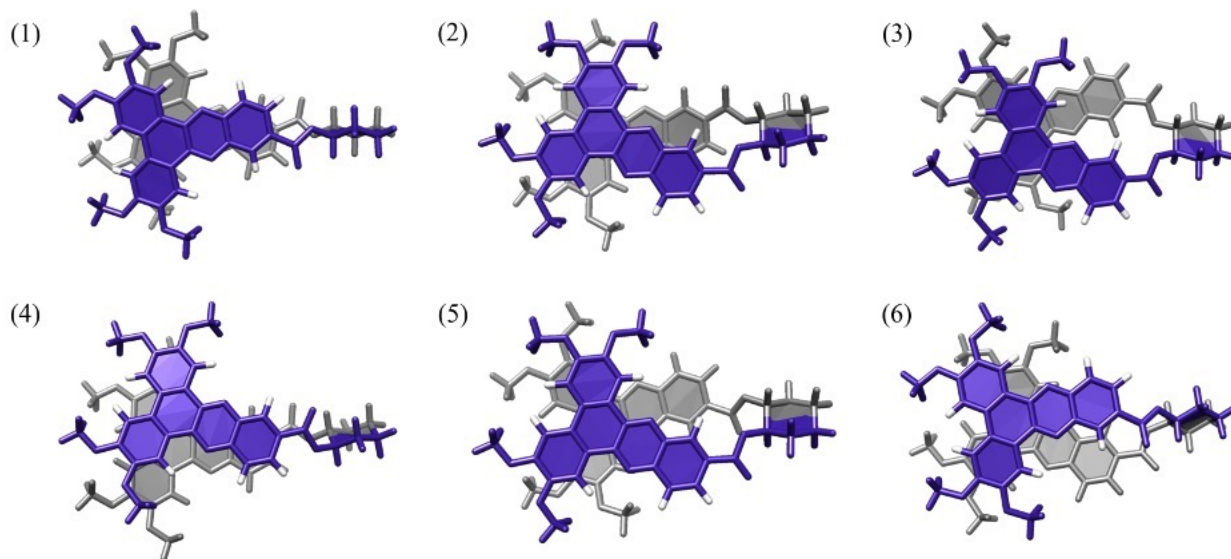
This section describes the total number of conformations, the relative energy of each conformation, ΔE , the geometry of each conformation, and the observed $\Delta\delta$ versus calculated $\Delta\delta$ ^1H NMR fits for each folded conformation of **dDBP(trans)** and **dDBP(cis)**. The ΔE for each conformation is proportionate to the lowest energy conformation; the lowest energy conformation for each dimer is set at 0 kcal/mol. For each experimental $\Delta\delta$ versus calculated $\Delta\delta$ ^1H 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 S35, 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(trans)

Twenty conformations were analyzed for **dDBP(trans)**. The 20 conformations arise from the following geometrical factors: there are two possible chair conformers – both esters are equatorial (**dEq**) or both esters are axial (**dAx**). There are three configurations between the two esters and the cyclohexyl linker – both carbonyls are syn (**+1**), one carbonyl is syn and the other carbonyl is anti (**0**), or both carbonyls are anti (**-1**) to the methine hydrogens on the adjacent carbons of the cyclohexane ring. Finally, there are three configurations between the two esters and the DBP core – both carbonyls are syn (**+1**), one carbonyl is syn and the other carbonyl is anti (**0**), or both carbonyls are anti (**-1**) to H_a on the DBP core (see Figure S33 for schematic of the DBP core).

Table S6. The total number of conformations, energies, relative energies, number of imaginary frequencies, and R^2 fit and slope from the experimental $\Delta\delta$ versus calculated $\Delta\delta$ plots for each conformer of **dDBP(trans)**. The conformer with the best R^2 is bolded. *Carbonyl syn to the methine H is anti to H_a ; **carbonyl anti to the methine H is anti to H_a .

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq	NMR R^2 Fit	Slope
1	(dEq, +1, +1)	-3284.7887	+4.8	0	0.28	0.08
2	(dEq, +1, 0)	-3284.7932	+2.0	0	0.77	0.33
3	(dEq, +1, -1)	-3284.7961	+0.2	0	0.69	0.05
4	(dEq, 0, +1)	-3284.7813	+9.4	0	0.25	0.22
5	(dEq, 0, 0)*	-3284.7929	+2.2	0	0.33	0.06
6	(dEq, 0, 0)**	-3284.7937	+1.7	0	0.14	0.04
7	(dEq, 0, -1)	-3284.7832	+8.2	0	0.43	0.32
8	(dEq, -1, +1)	-3284.7708	+16.0	0	0.17	0.03
9	(dEq, -1, 0)	-3284.7790	+10.9	0	0.33	0.14
10	(dEq, -1, -1)	-3284.7963	0.0	0	0.54	0.06
11	(dAx, +1, +1)	-3284.7377	+36.8	0	0.00	0.03
12	(dAx, +1, 0)	-3284.7383	+36.4	0	0.18	1.06
13	(dAx, +1, -1)	-3284.7387	+36.2	0	0.10	0.40
14	(dAx, 0, +1)	-3284.7275	+43.2	0	0.02	-0.09
15	(dAx, 0, 0)*	-3284.7280	+42.9	1	0.14	-0.74
16	(dAx, 0, 0)**	-3284.7278	+43.0	0	0.26	0.98
17	(dAx, 0, -1)	-3284.7282	+42.7	0	0.10	0.29
18	(dAx, -1, +1)	-3284.7238	+45.5	0	0.13	-0.25
19	(dAx, -1, 0)	-3284.7240	+45.4	0	0.06	-0.70
20	(dAx, -1, -1)	-3284.7243	+45.2	0	0.02	-0.08



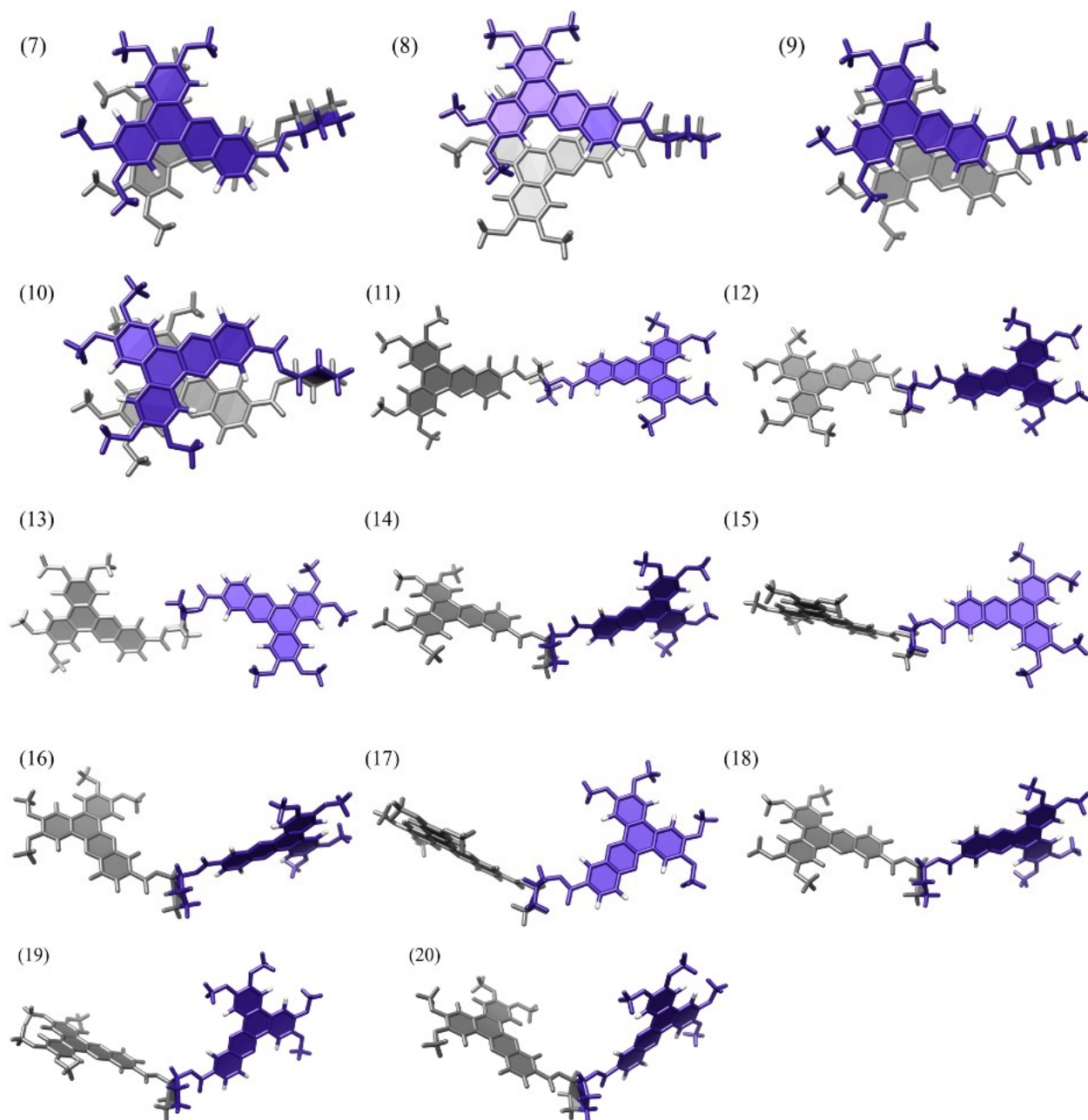
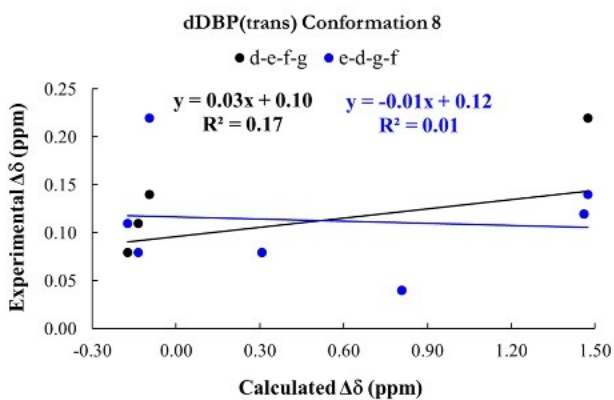
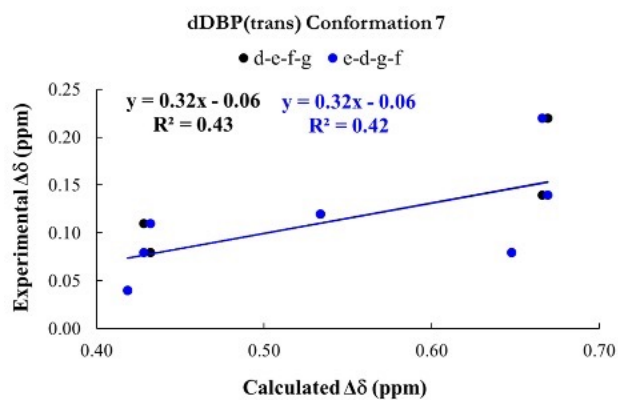
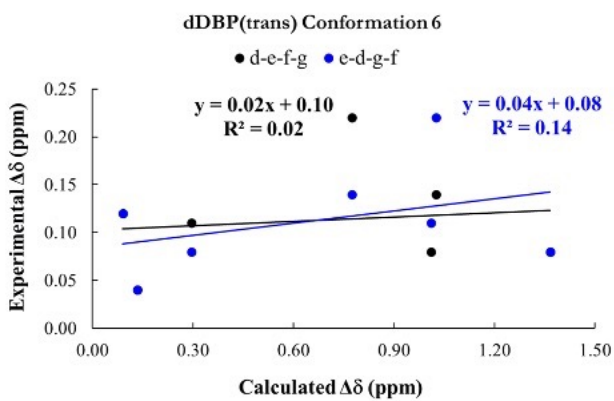
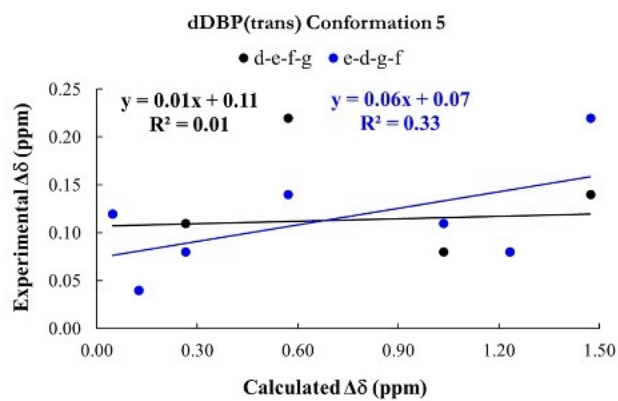
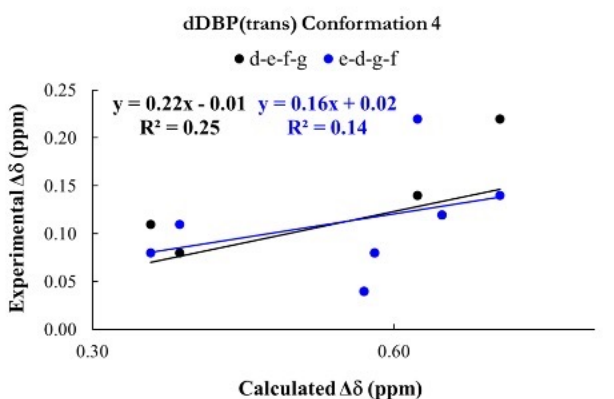
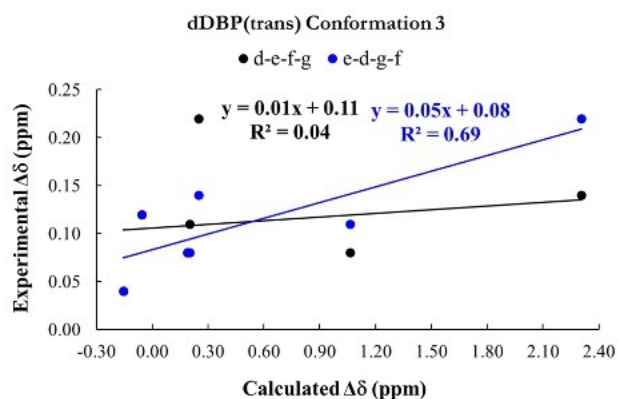
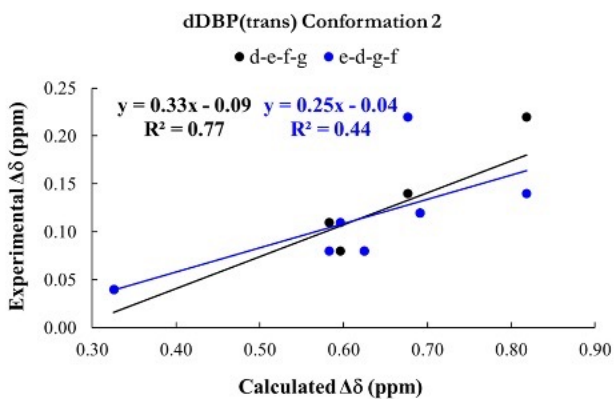
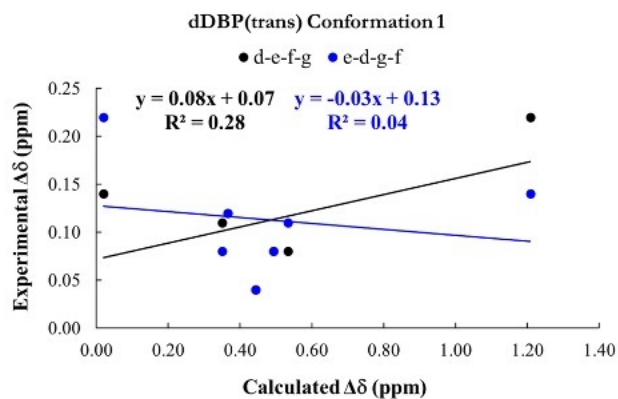
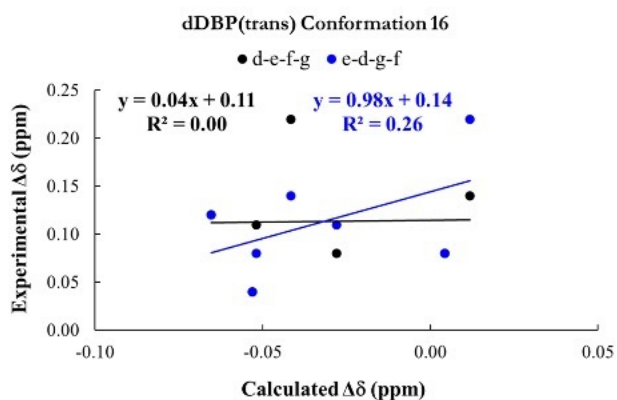
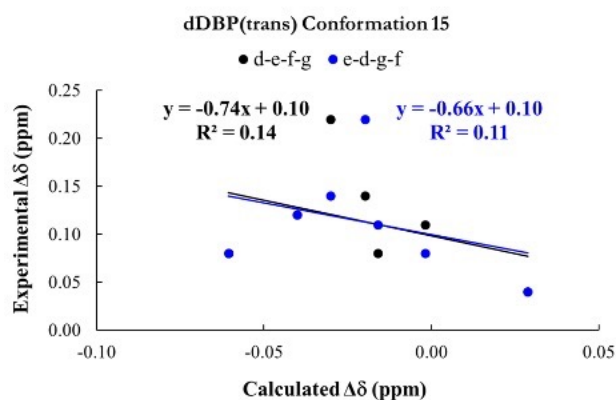
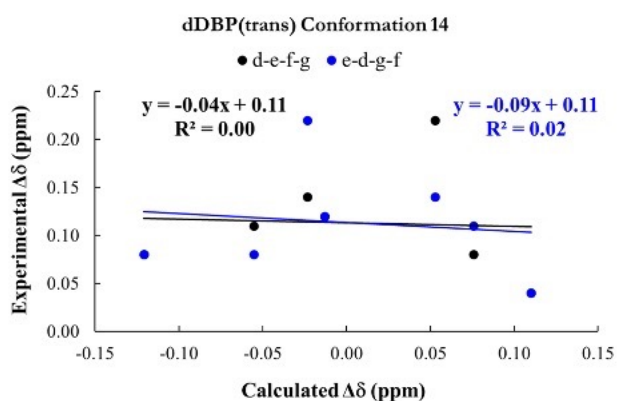
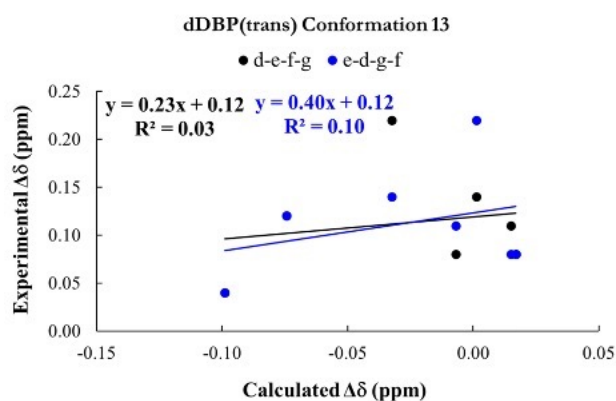
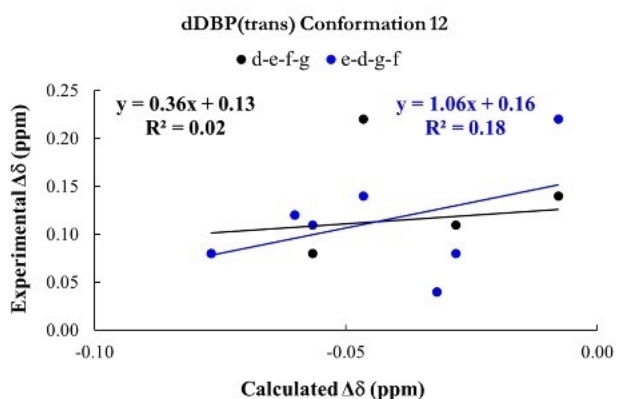
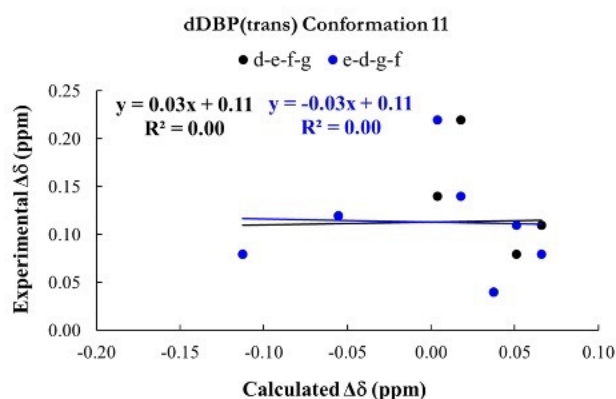
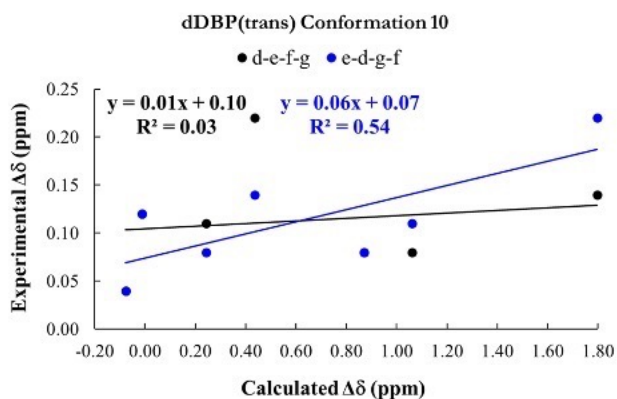
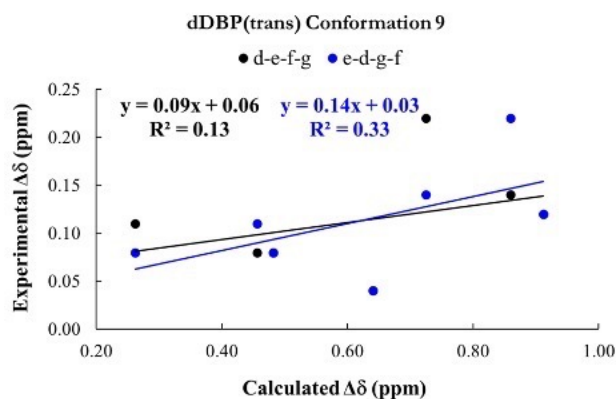


Figure S38. Schematics of all 20 conformations for **dDBP(trans)**. The number displayed in the figure corresponds to the conformation number in Table S6. For each conformation, the DBP core that appears in front is coloured in violet, and the other DBP core in the back is coloured in grey. Hydrogens on the DBP core in violet are shown in light grey.





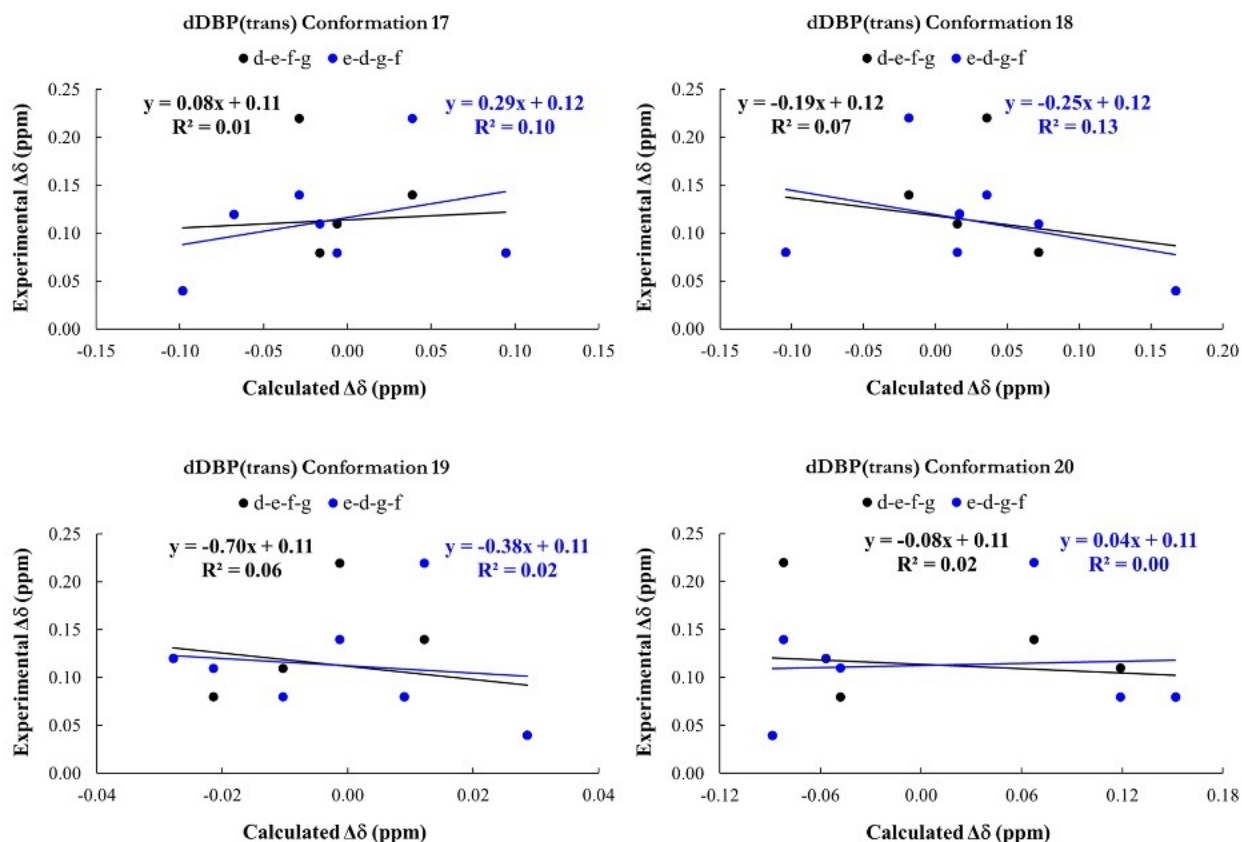


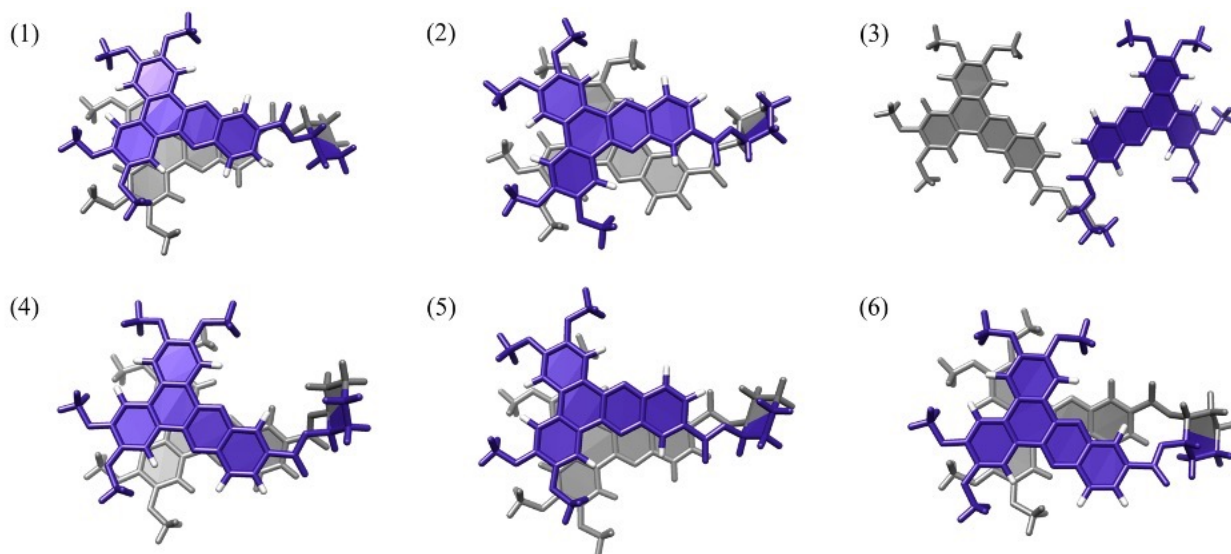
Figure S39. Experimental $\Delta\delta$ versus calculated $\Delta\delta$ NMR plots for each of the 20 conformations analyzed for **dDBP(trans)**. The title of each plot refers to the conformation number in Table S6 and Figure S38.

dDBP(cis)

Sixteen conformations were analyzed for **dDBP(cis)**. The 16 conformations arise from the following geometric factors: there is only one non-degenerate chair conformer, where one ester is in the equatorial position and the other is in the axial position. There are four configurations between the two esters and the methine proton of the cyclohexyl linker – both carbonyls are syn (**+3/2**), the equatorial carbonyl is anti and the axial carbonyl is syn (**+1/2**), the equatorial carbonyl is syn and the axial carbonyl is anti (**-1/2**), or both carbonyls are anti (**-3/2**) to the methine protons on the adjacent carbons of the cyclohexane ring. Finally, there are four configurations between the esters and the DBP core – both carbonyls are syn (**+3/2**), the equatorial carbonyl is anti and the axial carbonyl is syn (**+1/2**), the equatorial carbonyl is syn and the axial carbonyl is anti (**-1/2**), or both carbonyls are anti (**-3/2**) to H_a on the DBP core (see Figure S33 for schematic of the DBP core). Further attempts to optimize unfolded conformers were conducted under the same geometrical parameters listed above, yielding one additional conformation, number 17 in Table S7.

Table S7. The total number of conformations, energies, relative energies, number of imaginary frequencies, and R^2 fit and slope from the experimental $\Delta\delta$ versus calculated $\Delta\delta$ plots for each conformer of **dDBP(cis)**. The conformer with the best R^2 is bolded.

Number	Conformation	E (a.u.)	ΔE (kcal/mol)	Imaginary Freq	NMR R^2 Fit	Slope
1	(+3/2, +3/2)	-3284.7833	+8.7	0	0.04	0.17
2	(+3/2, +1/2)	-3284.7972	0.0	0	0.53	0.22
3	(+3/2, -1/2)	-3284.7424	+34.4	0	0.09	-1.08
4	(+3/2, -3/2)	-3284.7853	+7.5	0	0.23	0.65
5	(+1/2, +3/2)	-3284.7771	+12.6	0	0.60	0.18
6	(+1/2, +1/2)	-3284.7885	+5.5	0	0.59	0.50
7	(+1/2, -1/2)	-3284.7867	+6.6	0	0.43	0.53
8	(+1/2, -3/2)	-3284.7952	+1.3	0	0.89	0.16
9	(-1/2, +3/2)	-3284.7686	+18.0	0	0.39	-0.13
10	(-1/2, +1/2)	-3284.7755	+13.6	0	0.09	-0.21
11	(-1/2, -1/2)	-3284.7760	+13.3	0	0.09	-0.22
12	(-1/2, -3/2)	-3284.7920	+3.3	0	0.98	0.21
13	(-3/2, +3/2)	-3284.7668	+19.1	0	0.00	0.00
14	(-3/2, +1/2)	-3284.7821	+9.5	0	0.84	0.24
15	(-3/2, -1/2)	-3284.7815	+9.9	0	0.51	0.20
16	(-3/2, -3/2)	-3284.7684	+18.1	0	0.15	0.33
17 - unfolded	(+3/2, -1/2)	-3284.7408	+35.4	0	0.47	1.11



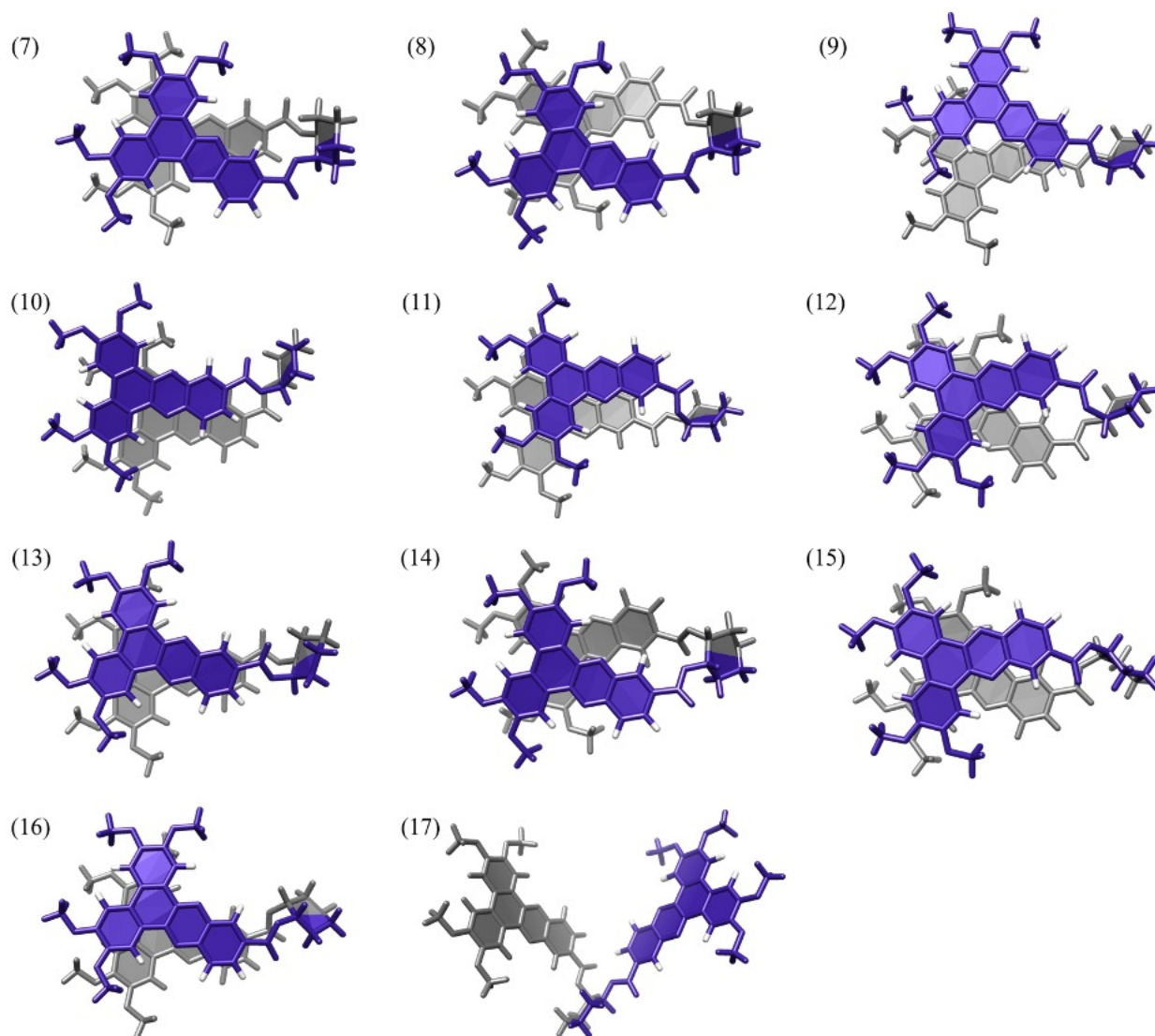
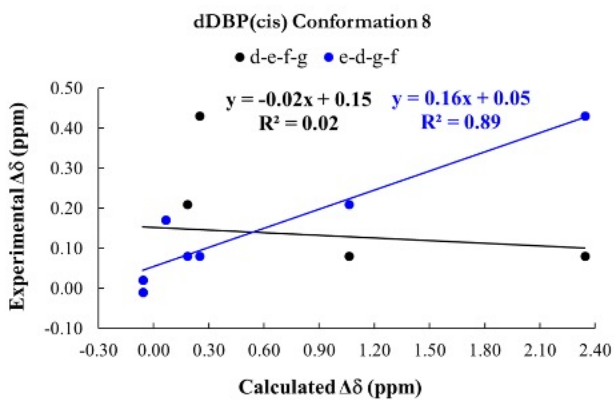
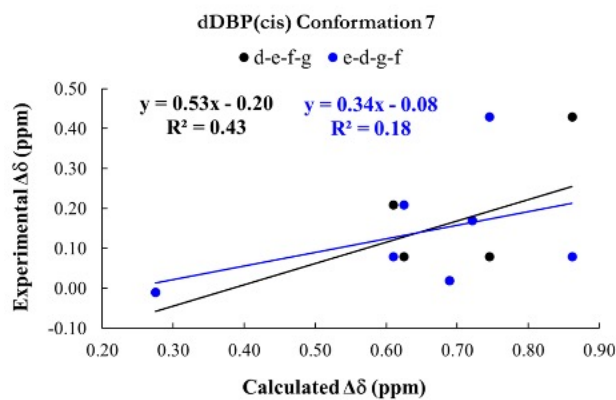
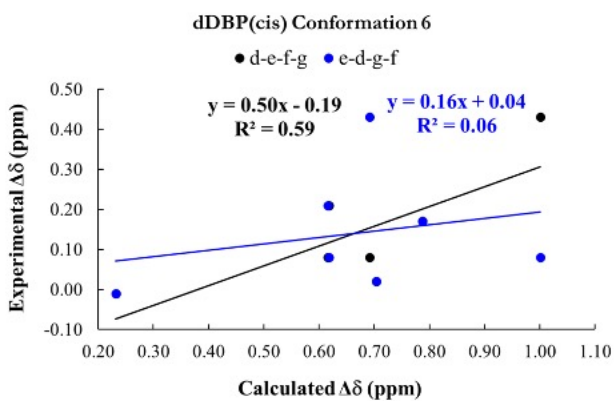
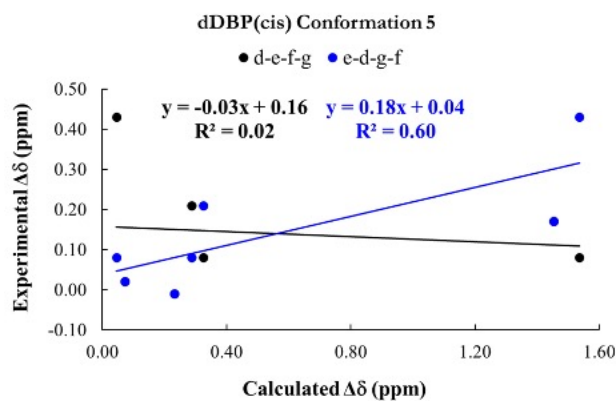
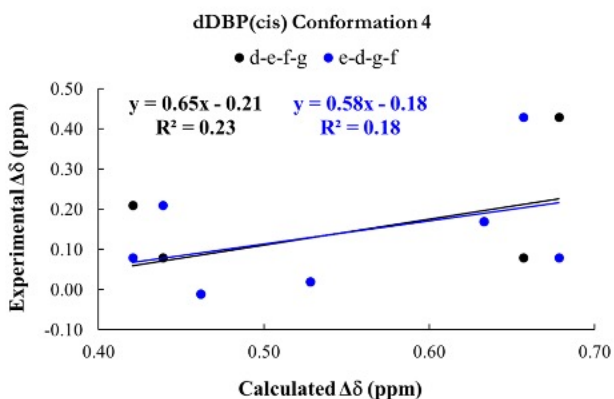
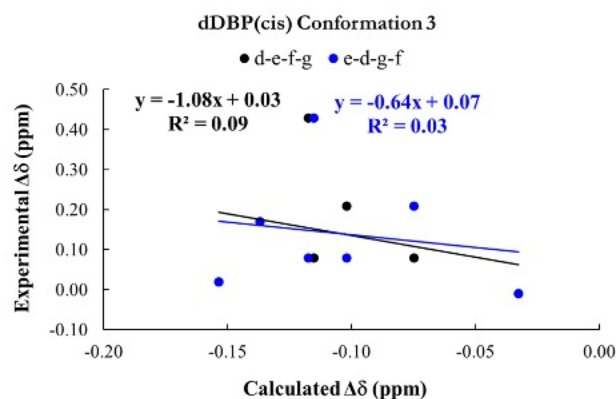
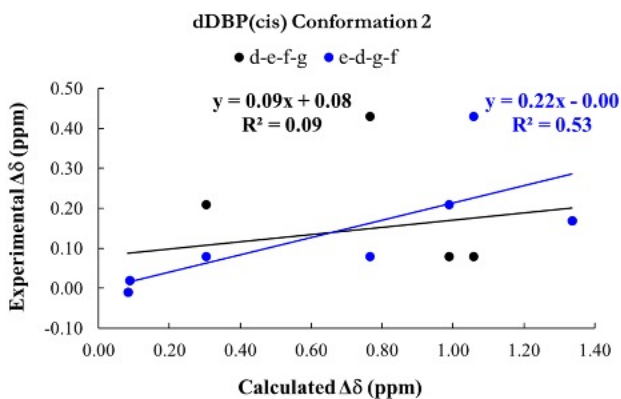
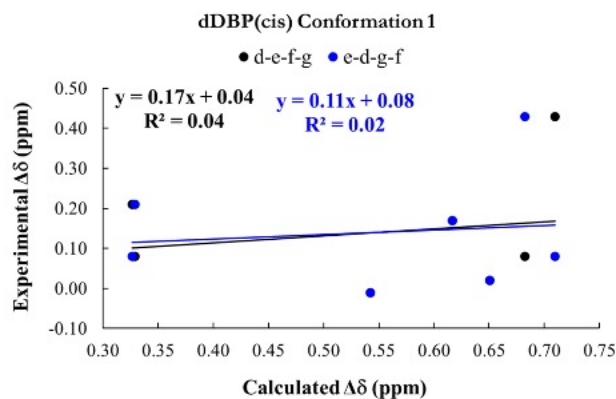
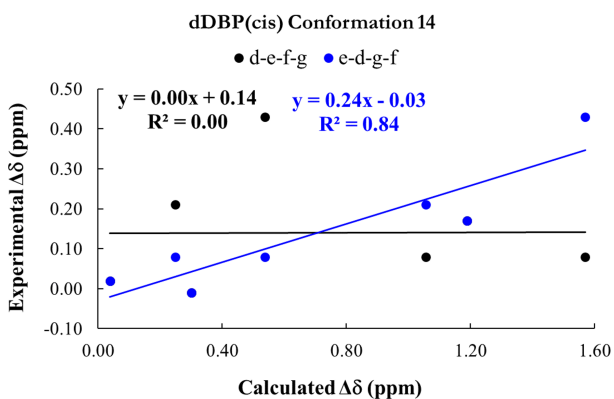
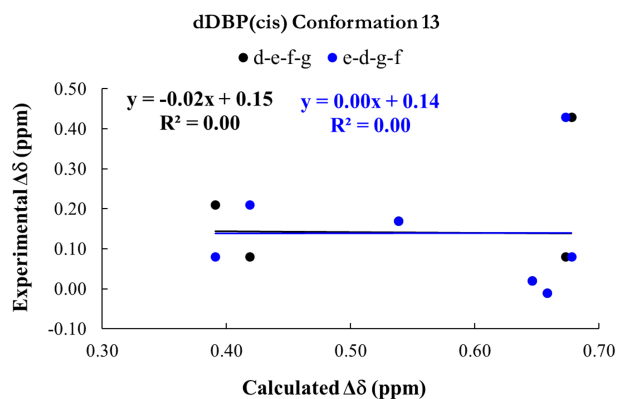
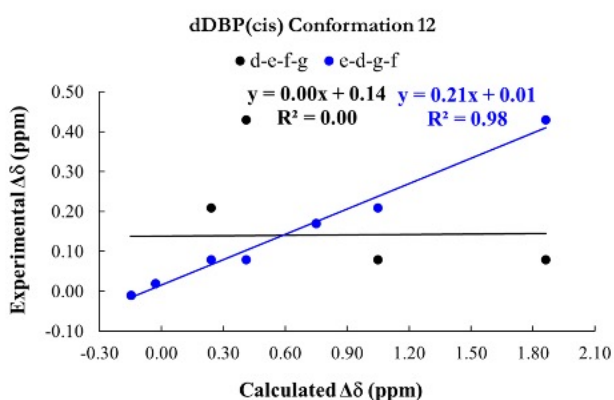
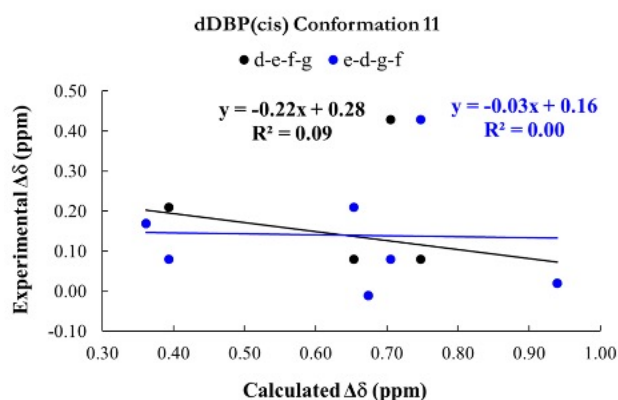
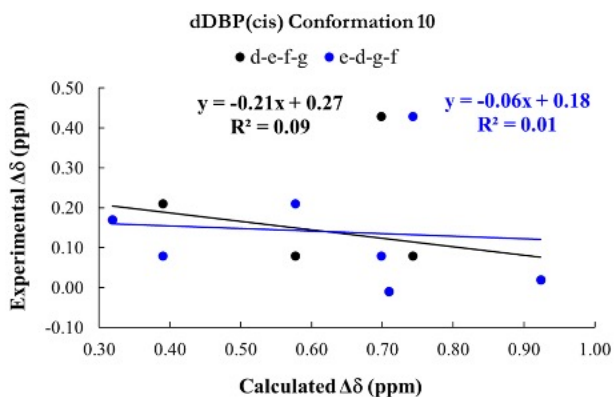
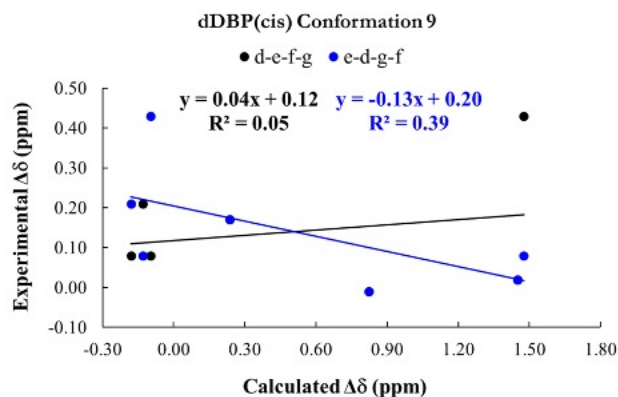


Figure S40. Schematics of all 17 conformations for **dDBP(cis)**. The number displayed in the figure corresponds to the conformation number in Table S7. For each conformation, the DBP core that appears in front is coloured in violet, and the other DBP core in the back is coloured in grey. Hydrogens on the DBP core in violet are shown in light grey.





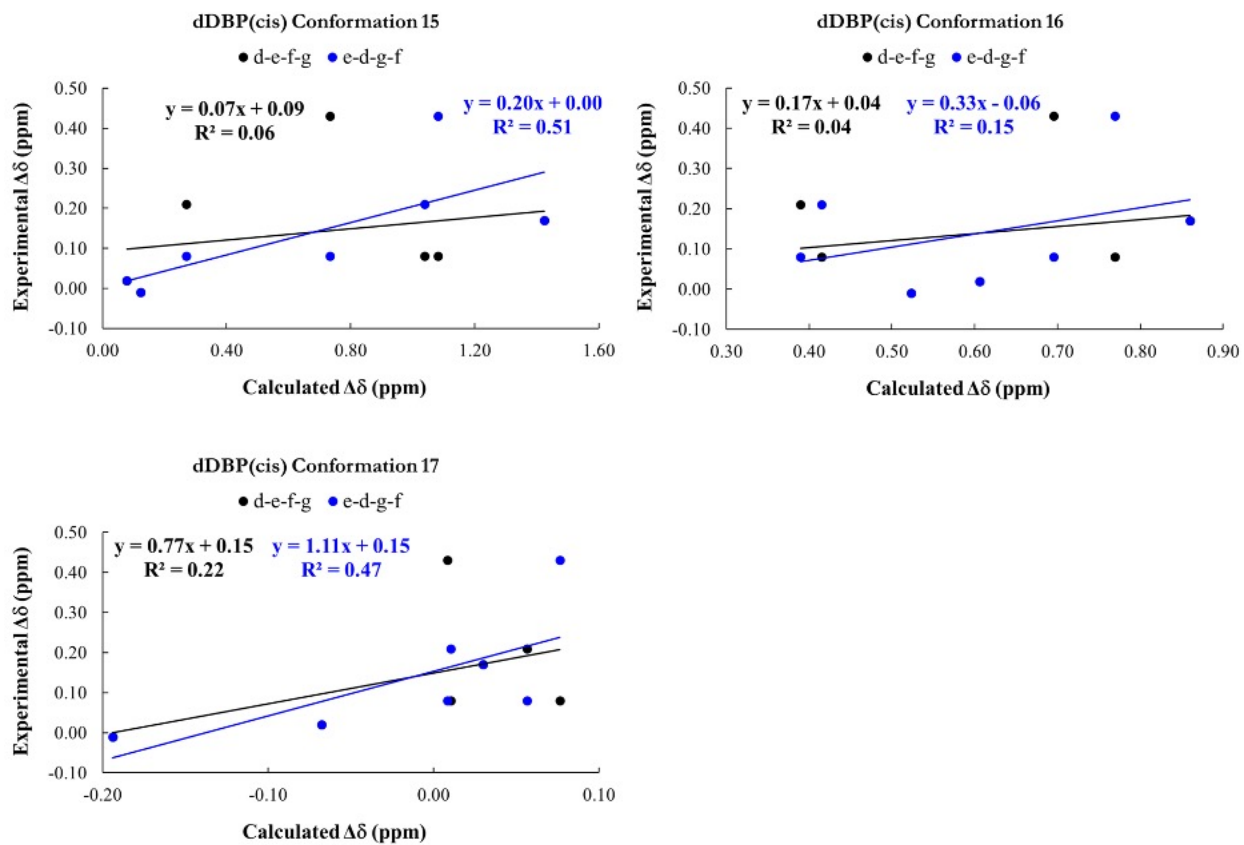


Figure S41. Experimental $\Delta\delta$ versus calculated $\Delta\delta$ NMR plots for each of the 17 conformations analyzed for **dDBP(cis)**. The title of each plot refers to the conformation number in Table S7 and Figure S40.

IV. Calculations with ORCA

Higher level DFT calculations were employed using the Grimme r2SCAN-3c variant with the recommended mTZVPP basis set.¹⁵ This functional has improved accuracy over the B3LYP-D3 functional for many applications, including noncovalent complexes. The calculations were performed on ORCA (version 5.0.3).¹⁶ Optimizations were performed on all folded structures and the lowest energy unfolded structure for both dimers, starting from geometries optimized by the B3LYP-D3 functional. The results of these calculations are summarized in Tables S8-S9 below. Our results show the geometries did not change significantly with the new functional; Figures S42-S43 show side-by-side comparisons for one optimized folded structure for each dimer.

Table S8. Results from optimizations of **dDBP(trans)** performed with the newer r2SCAN-3c functional. The energy, ΔE , is relative to the lowest energy conformer for each set of calculations. The bolded conformer is the structure that best fit the NMR data for each functional.

Conformation	E (a.u.) ^a	ΔE (kcal/mol) ^a	NMR fit ^a	E (a.u.) ^b	ΔE (kcal/mol) ^b	NMR fit ^b
1	-3284.7887	+4.8	0.28	-3284.0349	+3.6	0.29
2	-3284.7932	+2.0	0.77	-3284.0371	+2.2	0.47
3	-3284.7961	+0.2	0.69	-3284.0406	0.0	0.68
4	-3284.7813	+9.4	0.25	-3284.0277	+8.1	0.16
5	-3284.7929	+2.2	0.33	-3284.0352	+3.4	0.34
6	-3284.7937	+1.7	0.14	-3284.0356	+3.1	0.16
7	-3284.7832	+8.2	0.43	-3284.0293	+7.1	0.55
8	-3284.7708	+16.0	0.17	-3284.0207	+12.4	0.18
9	-3284.7790	+10.9	0.33	-3284.0263	+9.0	0.36
10	-3284.7963	0.0	0.54	-3284.0373	+2.1	0.53
Unfolded	-3284.7387	+36.2	N/A	-3284.0016	+24.5	N/A

^aB3LYP-D3 functional^{3,4,9} at the 6-31G(d) level; ^br2SCAN-3c functional¹⁵ at the mTZVPP level.

Table S9. Results from optimizations of **dDBP(cis)** performed with the newer r2SCAN-3c functional. The energy, ΔE , is relative to the lowest energy conformer for each set of calculations. The bolded conformer is the structure that best fit the NMR data for each functional.

Conformation	E (a.u.) ^a	ΔE (kcal/mol) ^a	NMR fit ^a	E (a.u.) ^b	ΔE (kcal/mol) ^b	NMR fit ^b
1	-3284.7833	+8.7	0.04	-3284.0301	+5.9	0.02
2	-3284.7972	0.0	0.53	-3284.0396	0.0	0.65
3	-3284.7424	+34.4	0.09	-3284.0038	+22.5	0.35
4	-3284.7853	+7.5	0.23	-3284.0316	+5.0	0.12
5	-3284.7771	+12.6	0.60	-3284.0235	+10.1	0.54
6	-3284.7885	+5.5	0.59	-3284.0309	+5.5	0.63
7	-3284.7867	+6.6	0.43	-3284.0281	+7.2	0.31
8	-3284.7952	+1.3	0.89	-3284.0393	+0.2	0.89
9	-3284.7686	+18.0	0.39	-3284.0222	+10.9	0.43
10	-3284.7755	+13.6	0.09	-3284.0222	+10.9	0.17
11	-3284.7760	+13.3	0.09	-3284.0223	+10.8	0.15
12	-3284.7920	+3.3	0.98	-3284.0325	+4.4	0.99
13	-3284.7668	+19.1	0.00	-3284.0108	+18.1	0.01
14	-3284.7821	+9.5	0.84	-3284.0234	+10.2	0.86
15	-3284.7815	+9.9	0.51	-3284.0216	+11.3	0.61
16	-3284.7684	+18.1	0.15	-3284.0124	+17.1	0.09
Unfolded	-3284.7408	+35.4	N/A	-3284.0022	+23.5	N/A

^aB3LYP-D3 functional^{3,4,9} at the 6-31G(d) level;⁵ ^br2SCAN-3c functional¹⁵ at the mTZVPP level.

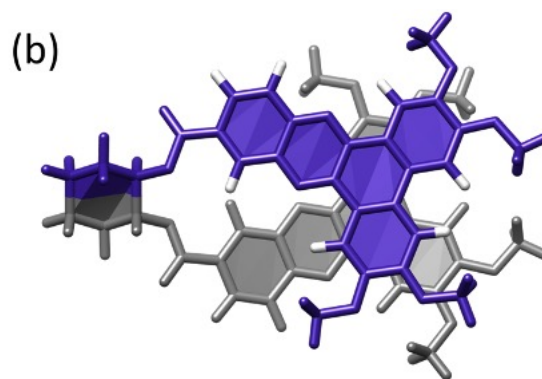
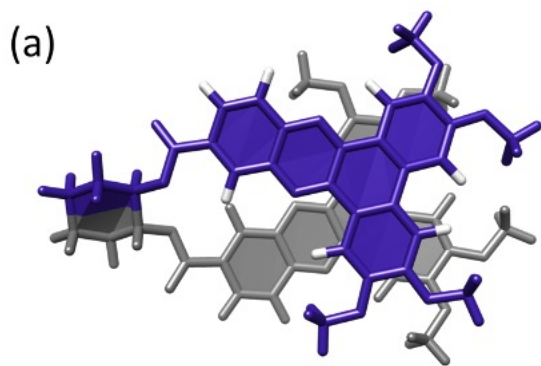


Figure S42. Optimized folded conformers (#3 in Table S8) of **dDBP(trans)** using the (a) B3LYP-D3 and (b) r2SCAN-3c functionals.

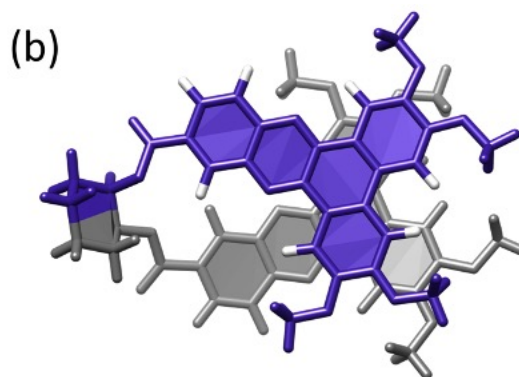
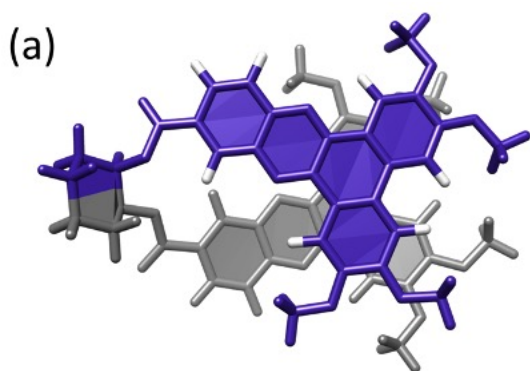


Figure S43. Optimized folded conformers (#8 in Table S9) of **dDBP(cis)** using the (a) B3LYP-D3 and (b) r2SCAN-3c functionals.

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(MeE) – lowest energy conformation with the B3LYP-D3 functional (#2 in Table S3).

```
Charge = 0 Multiplicity = 1
C      4.65052 -2.29594 -0.05165
C      3.29768 -2.65043 -0.06898
C      2.31683 -1.65665 -0.0438
C      2.68815 -0.30284 -0.00104
C      4.04068  0.05395  0.01583
C      5.03636 -0.9412  -0.00901
H      5.39404 -3.08276 -0.0716
H      3.01611 -3.69575 -0.10158
H      4.30916  1.10296  0.04864
C      0.39515  0.32412  0.00838
C      0.0249  -1.02937 -0.03402
C     -0.64156  1.38363  0.01889
C     -2.01264  1.03689 -0.00946
C     -0.25694  2.73529  0.03431
C     -2.96358  2.08099 -0.07222
C     -1.21528  3.76748  0.00474
H      0.7957  2.97457  0.06442
C     -2.57466  3.43927 -0.0564
H     -4.0076  1.85408 -0.15146
C     -1.40591 -1.41517 -0.03273
C     -2.41043 -0.42051  0.00591
C     -1.76056 -2.77493 -0.04633
C     -3.75926 -0.83742  0.07955
C     -3.1095  -3.17793 -0.00453
H     -0.97539 -3.5152  -0.08429
C     -4.11356 -2.20532  0.06586
H     -4.54297 -0.11202  0.16606
N      0.99942 -1.98209 -0.05798
N      1.71948  0.64819  0.02262
O     -3.52155 -4.52988 -0.01815
O     -5.44814 -2.66853  0.12362
O     -3.49023  4.51577 -0.1024
O     -0.88455  5.14154  0.02217
C     -2.52251 -5.54748 -0.08786
H     -1.93512 -5.45424 -1.0265
H     -1.85863 -5.50423  0.80215
H     -3.02219 -6.53772 -0.09368
C     -6.50621 -1.71165  0.17964
H     -7.47417 -2.25259  0.20669
H     -6.43077 -1.10006  1.10419
```

H	-6.49871	-1.06757	-0.72584
C	-4.88802	4.22809	-0.14756
H	-5.14127	3.66646	-1.07221
H	-5.20057	3.66551	0.75833
H	-5.44834	5.18518	-0.16592
C	0.49277	5.51184	0.08682
H	0.56382	6.61868	0.09853
H	0.9567	5.12852	1.02092
H	1.03842	5.1432	-0.80816
C	6.46812	-0.56535	0.01056
O	7.35286	-1.46827	-0.00921
O	6.82454	0.79517	0.05216
C	8.22597	1.06662	0.07187
H	8.37932	2.16474	0.10487
H	8.69604	0.62034	0.97493
H	8.71163	0.67283	-0.84723

mDBP(trans) – lowest energy conformation with the B3LYP-D3 functional (#6 in Table S4).

Charge = 0 Multiplicity = 1

C	6.82269	1.55901	1.35399
C	7.28327	0.09633	1.40691
C	6.8434	-0.68295	0.15537
C	7.33451	0.01583	-1.13194
C	6.88429	1.48662	-1.17265
C	7.32829	2.24909	0.08266
H	7.32643	-1.68305	0.20517
H	8.39128	0.06155	1.4991
H	6.85629	-0.38922	2.31097
H	5.71208	1.60621	1.38934
H	7.2142	2.09819	2.2433
H	6.88701	-0.50125	-2.01299
H	7.31283	1.98017	-2.07172
H	5.77653	1.53523	-1.26069
H	8.43812	2.31615	0.10957
H	6.92607	3.28424	0.04365
O	5.40807	-0.76032	0.1306
O	8.73568	-0.04677	-1.22037
H	8.96602	-0.97623	-1.48274
C	4.79701	-2.02946	0.1362
O	5.48218	-3.09047	0.14651
C	2.67087	-3.36581	0.11186
C	1.27437	-3.44345	0.09031
C	0.51184	-2.27355	0.07345
C	1.14646	-1.02083	0.07894
C	2.54255	-0.9405	0.10082
C	3.31947	-2.11455	0.11663
H	3.24232	-4.28544	0.12402
H	0.78951	-4.41189	0.08598
H	3.0148	0.0347	0.10446

C	-0.97425	0.05203	0.03839
C	-1.60818	-1.20014	0.0328
N	0.38786	0.10459	0.06158
N	-0.84407	-2.32911	0.0505
C	-1.77641	1.29787	0.0207
C	-1.12579	2.54357	0.02839
C	-3.18971	1.23478	-0.00176
C	-1.85481	3.74833	0.01642
H	-0.04626	2.56478	0.04396
C	-3.91032	2.45173	-0.00768
C	-3.25345	3.70286	0.00002
H	-4.98082	2.44535	-0.01612
C	-3.08703	-1.29093	0.00407
C	-3.70603	-2.55266	-0.00725
C	-3.87256	-0.11425	-0.01657
C	-5.10829	-2.67802	-0.04234
H	-3.08432	-3.4354	0.00998
C	-5.27943	-0.25363	-0.05508
C	-5.89904	-1.52364	-0.06745
H	-5.90736	0.61314	-0.07895
O	-1.25154	5.02654	0.0217
O	-3.93211	4.94334	-0.00785
O	-7.30018	-1.71056	-0.10537
O	-5.78148	-3.92078	-0.05605
C	0.17376	5.10922	0.03952
H	0.5804	4.64103	0.96162
H	0.6036	4.63576	-0.86925
H	0.46859	6.17854	0.04023
C	-5.35979	4.94673	-0.02018
H	-5.75939	4.45551	0.89284
H	-5.71314	5.99805	-0.02449
H	-5.74365	4.45303	-0.93867
C	-8.14716	-0.56162	-0.13649
H	-8.00822	0.051	0.77998
H	-7.95552	0.04015	-1.05071
H	-9.20359	-0.89849	-0.16477
C	-5.00498	-5.11872	-0.03499
H	-4.39996	-5.17554	0.89528
H	-5.69224	-5.98926	-0.04955
H	-4.35635	-5.17908	-0.93514

mDBP(cis) – lowest energy conformation with the B3LYP-D3 functional (#6 in Table S5).

Charge = 0 Multiplicity = 1

C	-7.35756	2.3242	-0.05407
C	-6.92618	1.50743	1.1699
C	-7.40546	0.05067	1.06046
C	-6.89788	-0.60478	-0.24223
C	-7.32333	0.22586	-1.46433

C	-6.85191	1.68201	-1.35073
H	-5.81811	1.5377	1.26525
H	-7.35839	1.9692	2.08399
H	-8.46703	2.39833	-0.08185
H	-6.9479	3.35382	0.02908
H	-7.39257	-1.59616	-0.33535
H	-6.89542	-0.22726	-2.38462
H	-8.43143	0.20402	-1.56115
H	-5.74083	1.72213	-1.37998
H	-7.23592	2.25962	-2.21891
H	-8.52148	0.0513	1.05846
O	-6.94422	-0.66877	2.17398
H	-7.4597	-1.51709	2.20012
O	-5.46313	-0.69363	-0.20853
C	-4.8633	-1.96754	-0.23758
O	-5.55787	-3.02206	-0.26592
C	0.92331	0.06435	-0.06944
C	-1.20542	-0.99062	-0.13954
C	-0.58116	-2.24855	-0.14023
C	1.54694	-1.19299	-0.06823
H	-3.06444	0.08059	-0.17106
C	-2.6004	-0.89853	-0.17323
C	-1.35317	-3.41189	-0.17642
C	-2.74879	-3.32239	-0.21068
C	-3.38679	-2.06576	-0.20793
H	-0.8763	-4.38425	-0.17708
H	-3.32781	-4.23699	-0.2375
C	1.73528	1.30338	-0.03615
C	3.14762	1.22868	0.00098
C	1.09488	2.55437	-0.04736
C	3.878	2.43967	0.0169
C	1.8334	3.75317	-0.02525
H	0.01582	2.58436	-0.07484
C	3.23129	3.69619	0.00631
H	4.94835	2.42431	0.03297
C	3.02458	-1.29597	-0.02343
C	3.81928	-0.12606	0.01715
C	3.63307	-2.56279	-0.01518
C	5.22426	-0.27736	0.07603
C	5.03362	-2.70007	0.03728
H	3.00456	-3.44016	-0.04884
C	5.83333	-1.5526	0.08427
H	5.85861	0.58399	0.12022
N	-0.43792	0.12828	-0.10493
N	0.77396	-2.31549	-0.10405
O	3.91981	4.93106	0.02484
O	1.24049	5.03626	-0.03576
O	7.23215	-1.75174	0.13927
O	5.69635	-3.94847	0.04796
C	-0.18373	5.13034	-0.07429
H	-0.63057	4.65993	0.82776
H	-0.47015	6.20194	-0.07856

H	-0.58068	4.66595	-1.00249
C	5.34704	4.92279	0.05956
H	5.75675	4.43143	-0.84887
H	5.70886	5.97121	0.07284
H	5.71256	4.42291	0.98225
C	8.08867	-0.6105	0.18552
H	7.96437	0.00829	-0.72903
H	7.89284	-0.01229	1.10118
H	9.14175	-0.95701	0.22311
C	4.91011	-5.13959	0.00789
H	4.31683	-5.18429	-0.93056
H	5.5898	-6.01596	0.02502
H	4.24921	-5.20103	0.89907

dDBP(trans) – lowest energy folded conformer with the r2SCAN-3c functional (#3 in Table S8).

Charge = 0 Multiplicity = 1

C	-4.2381	-2.4184	-1.0586
C	-3.4288	-1.321	-1.2653
C	-2.0343	-1.4911	-1.4181
C	-1.4833	-2.8096	-1.3664
C	-2.3501	-3.9216	-1.2315
C	-3.6919	-3.7291	-1.0659
H	-3.8306	-0.3139	-1.2679
H	-1.911	-4.9148	-1.2296
H	-4.3664	-4.5642	-0.9125
C	0.6251	-1.9384	-1.49
C	0.0712	-0.6139	-1.6148
C	2.0592	-2.1165	-1.4366
C	2.9144	-1.0108	-1.5896
C	2.5841	-3.3958	-1.1853
C	4.302	-1.2398	-1.5117
C	3.9398	-3.6023	-1.0878
H	1.8805	-4.2056	-1.0472
C	4.8157	-2.5003	-1.2735
H	4.9885	-0.4123	-1.6217
C	0.9638	0.5184	-1.773
C	2.3586	0.3213	-1.7889
C	0.4335	1.8162	-1.8967
C	3.1841	1.4467	-1.9671
C	1.2557	2.9114	-2.0385
H	-0.6433	1.922	-1.8619
C	2.6621	2.7177	-2.0903
H	4.2573	1.3268	-1.9907
N	-0.1541	-3.0062	-1.4004
N	-1.238	-0.4136	-1.572
O	3.396	3.8422	-2.2525
O	0.8444	4.1966	-2.1328
O	6.1366	-2.794	-1.1771

O	4.5335	-4.7867	-0.8099
C	-0.5608	4.4286	-2.1156
H	-0.6847	5.509	-2.1959
H	-1.0523	3.9387	-2.9656
H	-1.0102	4.0748	-1.181
C	4.8081	3.7048	-2.3579
H	5.2422	3.2896	-1.4405
H	5.0798	3.0783	-3.2176
H	5.1932	4.7139	-2.5071
C	7.0642	-1.7521	-1.4322
H	6.9322	-1.3364	-2.4395
H	6.972	-0.9436	-0.6947
H	8.0534	-2.2038	-1.3503
C	3.6701	-5.8891	-0.5406
H	4.3266	-6.7261	-0.3003
H	3.012	-5.6735	0.3102
H	3.0653	-6.1413	-1.4208
C	-5.6684	-2.2923	-0.687
O	-6.3222	-3.207	-0.2327
O	-6.1456	-1.0406	-0.8415
C	-7.3755	-0.746	-0.1403
C	-7.3756	0.7448	0.1399
C	-8.6084	-1.1302	-0.9455
H	-7.3618	-1.3007	0.8074
C	-8.6088	1.1287	0.945
H	-7.362	1.2995	-0.8078
C	-9.8766	-0.7436	-0.1809
H	-8.575	-0.6068	-1.9106
H	-8.5823	-2.2042	-1.1468
C	-9.8767	0.7419	0.1803
H	-8.5829	2.2028	1.1463
H	-8.5753	0.6054	1.9101
H	-10.7599	-0.9936	-0.7785
H	-9.9384	-1.343	0.7378
H	-10.7602	0.9917	0.7778
H	-9.9387	1.3413	-0.7384
O	-6.1459	1.0396	0.8412
C	-5.6689	2.2913	0.6867
O	-6.3228	3.2061	0.2325
C	0.0707	0.614	1.6161
C	-2.0349	1.4908	1.419
C	-1.4841	2.8095	1.3675
C	0.6244	1.9387	1.4913
H	-3.8309	0.3133	1.2681
C	-3.4293	1.3205	1.2658
C	-2.3511	3.9213	1.2326
C	-3.6928	3.7286	1.0666
C	-4.2387	2.4177	1.059
H	-1.9122	4.9146	1.2308
H	-4.3674	4.5636	0.9131
N	-0.155	3.0063	1.4017
N	-1.2384	0.4135	1.573

C	2.0584	2.1169	1.4375
C	2.5831	3.3962	1.1858
C	2.9139	1.0113	1.59
C	3.9388	3.6028	1.0876
H	1.8793	4.206	1.0481
C	4.3014	1.2404	1.5111
C	4.8148	2.501	1.2725
H	4.9879	0.4129	1.6206
C	0.9635	-0.5181	1.7742
C	0.4334	-1.816	1.898
C	2.3583	-0.3208	1.7898
C	1.2558	-2.9111	2.0398
H	-0.6433	-1.922	1.8635
C	3.184	-1.4461	1.9679
C	2.6622	-2.7172	2.0912
H	4.2571	-1.3259	1.9914
O	4.5322	4.7873	0.8092
O	6.1356	2.7947	1.1752
O	0.8447	-4.1963	2.1342
O	3.3963	-3.8415	2.2533
C	3.6685	5.8895	0.5401
H	4.3249	6.7265	0.2992
H	3.0099	5.6737	-0.3101
H	3.0643	6.142	1.4207
C	7.0635	1.7528	1.4291
H	8.0526	2.2044	1.346
H	6.9327	1.3369	2.4364
H	6.9704	0.9444	0.6915
C	4.8084	-3.704	2.3576
H	5.1938	-4.7132	2.5058
H	5.2418	-3.2882	1.44
H	5.0808	-3.078	3.2175
C	-0.5604	-4.4285	2.1172
H	-1.0101	-4.0746	1.1829
H	-0.6841	-5.509	2.1974
H	-1.0518	-3.9389	2.9675

dDBP(trans) – lowest energy unfolded conformer with the r2SCAN-3c functional (#13 in Table S8).

Charge = 0 Multiplicity = 1

C	0.1728	0.8716	2.3446
C	-0.3388	1.5139	1.0544
C	0.1479	0.7715	-0.1838
C	-0.1449	-0.7266	-0.1219
C	0.3249	-1.3596	1.1818
C	-0.204	-0.6093	2.4051
H	-0.2917	1.2015	-1.09
H	-1.436	1.491	1.0388
H	-0.0395	2.5637	0.9791

H	1.2649	0.9733	2.3965
H	-0.235	1.4068	3.2092
H	0.307	-1.2313	-0.9822
H	0.0256	-2.4123	1.1931
H	1.4221	-1.3376	1.1794
H	-1.2968	-0.7068	2.4499
H	0.1909	-1.0689	3.3179
O	1.5916	0.8514	-0.2841
O	-1.5867	-0.8182	-0.2329
C	2.0994	1.9729	-0.8395
C	-2.085	-1.9747	-0.7218
O	-1.3978	-2.9038	-1.0837
O	1.4196	2.8823	-1.2605
C	7.7596	-0.0303	-0.0172
C	5.7297	0.9419	-0.4302
C	6.3841	2.0813	-0.9956
C	8.4194	1.1191	-0.5845
H	3.8434	0.0325	0.0532
C	4.32	0.9058	-0.3773
C	5.5994	3.1508	-1.4921
C	4.2351	3.0912	-1.4301
C	3.5834	1.9611	-0.8691
H	6.1128	4.007	-1.9183
H	3.6189	3.9001	-1.8068
C	-7.7616	0.0146	0.0142
C	-5.7233	-0.9524	-0.3687
C	-6.3669	-2.1	-0.9299
C	-8.4102	-1.1391	-0.5571
H	-3.846	-0.0285	0.1218
C	-4.3144	-0.9092	-0.3026
C	-5.5727	-3.1737	-1.4017
C	-4.2095	-3.1095	-1.3218
C	-3.5684	-1.9685	-0.7709
H	-6.078	-4.0369	-1.8235
H	-3.5862	-3.9225	-1.6775
N	-7.7078	-2.1679	-1.0133
N	-6.442	0.0881	0.0971
N	6.4389	-0.098	0.0512
N	7.7262	2.1456	-1.0596
C	8.5503	-1.1352	0.4873
C	7.9048	-2.2593	1.0349
C	9.9548	-1.0839	0.4264
C	8.6225	-3.3283	1.52
H	6.8232	-2.2502	1.0576
C	10.6767	-2.1853	0.9262
C	10.042	-3.2885	1.4629
H	11.7564	-2.1788	0.8917
C	9.8653	1.16	-0.6386
C	10.509	2.2842	-1.1899
C	10.6221	0.082	-0.1418
C	11.8806	2.3598	-1.2562
H	9.882	3.085	-1.559

C	12.0253	0.1739	-0.2155
C	12.6553	1.2781	-0.7559
H	12.6353	-0.6349	0.1597
C	-9.8549	-1.1815	-0.637
C	-10.4874	-2.3062	-1.2003
C	-10.6215	-0.1039	-0.1548
C	-11.8574	-2.382	-1.2938
H	-9.8531	-3.1068	-1.5571
C	-12.023	-0.1961	-0.2563
C	-12.642	-1.3002	-0.8093
H	-12.6404	0.6133	0.1055
C	-8.5625	1.117	0.5079
C	-7.928	2.2415	1.0675
C	-9.9658	1.0618	0.4272
C	-8.6556	3.3064	1.5466
H	-6.8468	2.2353	1.1054
C	-10.6979	2.1591	0.9211
C	-10.0741	3.2621	1.4706
H	-11.7771	2.1486	0.8736
O	-12.5532	-3.417	-1.8185
O	-13.9781	-1.4551	-0.939
O	-10.7116	4.3479	1.9626
O	-8.1365	4.4265	2.1
O	12.5868	3.3949	-1.7667
O	13.9938	1.4332	-0.8578
O	10.6693	-4.3786	1.9583
O	8.0924	-4.4489	2.0619
C	6.6742	-4.5246	2.1323
H	6.2225	-4.481	1.1331
H	6.4498	-5.487	2.5929
H	6.2626	-3.7161	2.7499
C	12.0886	-4.3987	1.9232
H	12.4635	-4.339	0.893
H	12.5146	-3.5774	2.5144
H	12.384	-5.3522	2.3618
C	14.8216	0.3838	-0.3781
H	15.847	0.7086	-0.556
H	14.673	0.2171	0.6968
H	14.6356	-0.5517	-0.9218
C	11.8438	4.4949	-2.2761
H	11.1955	4.1869	-3.1064
H	11.2307	4.9584	-1.4927
H	12.582	5.2124	-2.6352
C	-6.7198	4.5055	2.1919
H	-6.5047	5.4666	2.6596
H	-6.3153	3.6956	2.8123
H	-6.2531	4.467	1.1993
C	-12.1304	4.3626	1.9107
H	-12.4928	4.3057	0.8759
H	-12.5601	3.5371	2.4934
H	-12.4348	5.313	2.3498
C	-14.8156	-0.4054	-0.4768

H	-14.6182	0.53	-1.0166
H	-15.8371	-0.7302	-0.6759
H	-14.6894	-0.2385	0.601
C	-11.7999	-4.5163	-2.3143
H	-11.1355	-4.2073	-3.1313
H	-11.2022	-4.9803	-1.5193
H	-12.5306	-5.2336	-2.6885

dDBP(cis) – lowest energy conformer with the r2SCAN-3c functional (#2 in Table S9).

Charge = 0 Multiplicity = 1

C	-4.3361	-2.1221	1.2022
C	-3.5123	-1.0268	1.3368
C	-2.1134	-1.1876	1.3683
C	-1.5443	-2.4936	1.264
C	-2.4161	-3.6019	1.1145
C	-3.774	-3.4207	1.0862
H	-3.9083	-0.0214	1.4142
H	-1.9785	-4.5926	1.0358
H	-4.4495	-4.262	0.9731
C	0.5529	-1.5925	1.4717
C	-0.0263	-0.2741	1.536
C	1.9917	-1.7365	1.589
C	2.8034	-0.5962	1.7583
C	2.5755	-3.016	1.5421
C	4.1878	-0.7898	1.9176
C	3.9354	-3.189	1.678
H	1.916	-3.861	1.3924
C	4.7535	-2.0482	1.8878
H	4.8299	0.0644	2.0765
C	0.8269	0.8902	1.6431
C	2.2191	0.7385	1.7486
C	0.2517	2.1724	1.6067
C	3.0069	1.9044	1.8189
C	1.0333	3.3005	1.652
H	-0.8232	2.2349	1.5045
C	2.4421	3.1633	1.7654
H	4.083	1.825	1.8729
N	-0.2083	-2.6705	1.321
N	-1.3363	-0.0961	1.489
C	-5.8144	-1.9702	1.148
O	-6.6084	-2.8767	1.0615
O	-6.1584	-0.6612	1.2114
O	0.5733	4.5734	1.5663
O	3.1311	4.3263	1.7856
O	6.078	-2.3041	2.0341
O	4.5891	-4.3716	1.6315
C	-0.8224	4.7327	1.3325
H	-1.1227	4.222	0.4091

H	-1.4131	4.345	2.172
H	-0.9879	5.8068	1.2379
C	4.5483	4.2583	1.8711
H	4.8968	5.2911	1.8577
H	4.8642	3.7744	2.8048
H	4.9739	3.7255	1.0125
C	6.9409	-1.2013	2.262
H	6.9188	-0.4935	1.4213
H	6.6785	-0.6703	3.1861
H	7.9433	-1.6203	2.3564
C	3.8132	-5.529	1.3331
H	4.52	-6.3589	1.3066
H	3.0637	-5.7144	2.1135
H	3.3219	-5.4279	0.3584
C	-7.5256	-0.2676	0.9899
C	-7.6814	1.0808	1.6759
C	-7.7964	-0.201	-0.5202
H	-8.1998	-1.0184	1.4229
C	-9.0349	1.7174	1.3621
H	-6.8755	1.7382	1.3261
H	-7.5454	0.9488	2.7548
C	-9.1027	0.5089	-0.8343
H	-7.7965	-1.2109	-0.9372
C	-9.223	1.867	-0.1464
H	-9.1074	2.6904	1.8601
H	-9.8428	1.0936	1.771
H	-9.1973	0.599	-1.9218
H	-9.9194	-0.1447	-0.4983
H	-10.1983	2.312	-0.372
H	-8.4603	2.5484	-0.5446
O	-6.6952	0.5345	-1.1175
C	-5.6988	-0.2423	-1.6157
O	-5.8358	-1.4126	-1.8913
C	-4.2419	1.8647	-1.5288
C	-2.9915	2.4293	-1.53
C	-1.8351	1.6223	-1.6783
C	-2.0042	0.2154	-1.8595
C	-3.2971	-0.3331	-1.9055
C	-4.4009	0.4672	-1.7207
H	-5.1216	2.4818	-1.3832
H	-2.8584	3.4998	-1.4045
H	-3.4103	-1.4047	-2.0283
C	0.2586	-0.077	-1.8426
C	0.4387	1.3473	-1.7136
C	1.404	-0.96	-1.8363
C	2.7025	-0.4323	-1.7541
C	1.1968	-2.3502	-1.8531
C	3.7784	-1.3396	-1.6879
C	2.2527	-3.2231	-1.7693
H	0.1747	-2.701	-1.8939
C	3.5731	-2.7057	-1.6881
H	4.7897	-0.9717	-1.5904

C	1.7851	1.8823	-1.6649
C	1.9828	3.271	-1.557
C	2.8939	1.0117	-1.7081
C	3.2477	3.8134	-1.5073
H	1.1025	3.8983	-1.5036
C	4.18	1.5816	-1.6799
C	4.3685	2.9462	-1.589
H	5.0465	0.9388	-1.7401
N	-0.9468	-0.6112	-1.9366
N	-0.6026	2.1678	-1.6306
O	2.1461	-4.5733	-1.7204
O	4.5456	-3.6385	-1.5869
O	5.5781	3.5593	-1.557
O	3.5378	5.1283	-1.3838
C	2.4391	6.0201	-1.2173
H	2.8787	7.0123	-1.1094
H	1.7826	6.0067	-2.097
H	1.864	5.7686	-0.3182
C	6.7341	2.7416	-1.6492
H	6.796	2.0379	-0.8073
H	6.7538	2.1789	-2.5914
H	7.5853	3.4223	-1.6153
C	5.8891	-3.1911	-1.466
H	6.0257	-2.5809	-0.5654
H	6.4957	-4.0927	-1.3797
H	6.1979	-2.623	-2.3536
C	0.8263	-5.1081	-1.6584
H	0.2826	-4.7069	-0.7934
H	0.2645	-4.8898	-2.5751
H	0.9477	-6.1873	-1.5567

dDBP(cis) – second lowest energy conformer with the r2SCAN-3c functional (#8 in Table S9).

Charge = 0 Multiplicity = 1

C	4.2041	-2.3045	1.5729
C	3.3495	-1.2226	1.6046
C	1.9565	-1.4251	1.7062
C	1.4458	-2.7605	1.7198
C	2.351	-3.8491	1.7558
C	3.6984	-3.625	1.6926
H	3.7176	-0.2051	1.5354
H	1.9414	-4.8535	1.806
H	4.4075	-4.4457	1.6969
C	-0.6865	-1.9448	1.6237
C	-0.1782	-0.6011	1.7411
C	-2.1047	-2.1594	1.4389
C	-2.997	-1.0743	1.5004
C	-2.5714	-3.4522	1.1459
C	-4.3646	-1.338	1.2922
C	-3.9055	-3.6917	0.915

H	-1.8379	-4.2448	1.0816
C	-4.8222	-2.6117	1.012
H	-5.0785	-0.5272	1.3307
C	-1.1092	0.5074	1.8256
C	-2.4953	0.2727	1.7414
C	-0.6234	1.8186	1.9844
C	-3.3612	1.3758	1.8546
C	-1.4823	2.8917	2.0622
H	0.45	1.952	2.0269
C	-2.8829	2.6611	2.0089
H	-4.43	1.2267	1.8055
N	0.1223	-2.9933	1.6576
N	1.1246	-0.3644	1.7589
C	5.6636	-2.1577	1.3375
O	6.4754	-3.0448	1.484
O	5.966	-0.9273	0.8781
O	-1.1124	4.1874	2.1841
O	-3.6557	3.7667	2.1076
O	-6.1199	-2.9385	0.7897
O	-4.4393	-4.8892	0.5787
C	0.284	4.4553	2.271
H	0.7227	3.9795	3.1572
H	0.8091	4.1112	1.3734
H	0.3742	5.5387	2.3566
C	-5.0677	3.5934	2.0939
H	-5.4901	4.5941	2.189
H	-5.409	3.1504	1.1507
H	-5.3966	2.9745	2.939
C	-7.0944	-1.9211	0.9513
H	-7.0675	-1.4982	1.9638
H	-6.9569	-1.113	0.2201
H	-8.0593	-2.3998	0.781
C	-3.5248	-5.9659	0.3836
H	-4.1321	-6.8161	0.0709
H	-2.7932	-5.7208	-0.3958
H	-3.0025	-6.2147	1.3161
C	7.285	-0.7202	0.3243
C	7.4185	-1.4214	-1.0227
C	7.4458	0.789	0.2014
H	8.0376	-1.1035	1.0263
C	8.7501	-1.0605	-1.6849
H	6.5863	-1.1015	-1.6618
H	7.3361	-2.5016	-0.8765
C	8.748	1.1566	-0.4973
H	7.3944	1.2613	1.189
C	8.8919	0.4522	-1.8458
H	8.8222	-1.5605	-2.6568
H	9.5789	-1.4438	-1.0725
H	8.7925	2.2448	-0.5997
H	9.5742	0.8617	0.1645
H	9.8601	0.7037	-2.2921
H	8.1189	0.82	-2.5324

O	6.2945	1.2302	-0.5609
C	5.7871	2.4398	-0.2559
O	6.4005	3.2996	0.3383
C	3.7914	3.8673	-0.6485
C	2.4539	4.0346	-0.8736
C	1.6206	2.9092	-1.0915
C	2.2034	1.6048	-1.1442
C	3.5934	1.4627	-0.9404
C	4.3684	2.5708	-0.6697
H	4.4368	4.7122	-0.4338
H	1.9927	5.0177	-0.8636
H	4.0203	0.4659	-0.9506
C	0.1331	0.6827	-1.463
C	-0.4559	1.9947	-1.3697
C	-0.7216	-0.4706	-1.6699
C	-2.1132	-0.3024	-1.805
C	-0.1579	-1.7596	-1.7233
C	-2.8978	-1.4457	-2.045
C	-0.9442	-2.8727	-1.9195
H	0.9132	-1.8435	-1.5907
C	-2.3426	-2.7073	-2.107
H	-3.9664	-1.3477	-2.1685
C	-1.8936	2.1419	-1.4299
C	-2.4657	3.4075	-1.214
C	-2.7097	1.0193	-1.6584
C	-3.8292	3.5845	-1.2262
H	-1.7934	4.2305	-1.012
C	-4.1032	1.2195	-1.6966
C	-4.6623	2.4665	-1.4932
H	-4.7598	0.3784	-1.8674
N	1.4419	0.5117	-1.3509
N	0.2916	3.0773	-1.2083
O	-0.5034	-4.1513	-1.9529
O	-3.0361	-3.8473	-2.3284
O	-5.9932	2.7304	-1.5027
O	-4.4695	4.7524	-0.9856
C	-3.6557	5.869	-0.6338
H	-4.3479	6.689	-0.4394
H	-3.0656	5.6561	0.266
H	-2.9861	6.1449	-1.4583
C	-6.8745	1.665	-1.818
H	-6.6605	1.2483	-2.8106
H	-6.8153	0.8625	-1.0704
H	-7.8777	2.0925	-1.8101
C	-4.4316	-3.7369	-2.5824
H	-4.6213	-3.1203	-3.4706
H	-4.7815	-4.7538	-2.7622
H	-4.967	-3.323	-1.7195
C	0.8979	-4.3577	-1.8051
H	1.4566	-3.8641	-2.6104
H	1.2544	-3.9918	-0.8355
H	1.0471	-5.4363	-1.8655

dDBP(cis) – folded conformer that best fit the NMR data with the r2SCAN-3c functional (#12 in Table S9).

Charge = 0 Multiplicity = 1

C	-4.1995	2.332	-1.1986
C	-3.3965	1.2282	-1.3895
C	-1.9964	1.3827	-1.4866
C	-1.4276	2.6921	-1.4079
C	-2.2843	3.8111	-1.2663
C	-3.634	3.6336	-1.1485
H	-3.8099	0.2268	-1.4319
H	-1.836	4.7998	-1.2394
H	-4.3023	4.4755	-1.0057
C	0.6709	1.7938	-1.542
C	0.0979	0.476	-1.6506
C	2.1095	1.9501	-1.5217
C	2.9439	0.8243	-1.6526
C	2.6638	3.2275	-1.3277
C	4.336	1.0315	-1.6107
C	4.0254	3.413	-1.2648
H	1.979	4.0561	-1.2052
C	4.8772	2.2886	-1.4259
H	5.0056	0.1895	-1.712
C	0.9691	-0.676	-1.7679
C	2.3663	-0.5065	-1.7878
C	0.4118	-1.9665	-1.8326
C	3.1702	-1.6562	-1.9024
C	1.2115	-3.0826	-1.9103
H	-0.6664	-2.0487	-1.7909
C	2.6219	-2.9211	-1.96
H	4.2461	-1.561	-1.9179
N	-0.0949	2.8711	-1.4402
N	-1.214	0.2945	-1.6241
C	-5.6556	2.2175	-0.9446
O	-6.3408	3.1372	-0.5502
O	-6.1309	0.9733	-1.1678
O	0.7732	-4.3631	-1.9318
O	3.3306	-4.0693	-2.0447
O	6.2056	2.5572	-1.3605
O	4.6468	4.5945	-1.0441
C	-0.6354	-4.5624	-1.8607
H	-1.0466	-4.1383	-0.9375
H	-1.1425	-4.1166	-2.7257
H	-0.7835	-5.6429	-1.8695
C	4.7482	-3.9729	-2.1104
H	5.1124	-4.9983	-2.1772
H	5.064	-3.4123	-3.0001
H	5.1605	-3.5061	-1.208
C	7.1067	1.4778	-1.5463
H	6.9882	0.7167	-0.7622
H	6.9712	1.0064	-2.5282
H	8.1068	1.908	-1.484

C	3.8116	5.7234	-0.7961
H	4.4902	6.5561	-0.6077
H	3.1878	5.9521	-1.6696
H	3.1756	5.5545	0.0811
C	-7.468	0.7044	-0.6935
C	-8.043	-0.4467	-1.4961
C	-7.4406	0.4982	0.8305
H	-8.0847	1.5978	-0.8621
C	-9.4549	-0.7521	-0.99
H	-7.4092	-1.3325	-1.4056
H	-8.0648	-0.1528	-2.5518
C	-8.7513	-0.1004	1.3566
H	-7.3201	1.4854	1.2855
C	-9.4426	-1.1541	0.4851
H	-9.9001	-1.5503	-1.5934
H	-10.0877	0.1372	-1.13
H	-8.5791	-0.4755	2.3714
H	-9.4308	0.7572	1.4613
H	-10.4712	-1.2793	0.8445
H	-8.9391	-2.1152	0.5904
O	-6.1939	-0.1223	1.2676
C	-5.8852	-1.4089	1.0499
O	-6.6669	-2.2664	0.6996
C	-4.0288	-3.0413	1.2181
C	-2.7064	-3.3737	1.3085
C	-1.7235	-2.3615	1.4317
C	-2.1357	-0.9951	1.5144
C	-3.5105	-0.68	1.4392
C	-4.4404	-1.6834	1.2714
H	-4.7922	-3.8014	1.0946
H	-2.3764	-4.4078	1.2778
H	-3.8052	0.3623	1.4842
C	0.0518	-0.3376	1.6552
C	0.4666	-1.7131	1.5454
C	1.052	0.7053	1.7656
C	2.4201	0.3741	1.7813
C	0.6492	2.0516	1.8322
C	3.3526	1.4225	1.8939
C	1.5736	3.0671	1.9085
H	-0.4125	2.2577	1.794
C	2.9558	2.7426	1.9542
H	4.4103	1.2038	1.9071
C	1.8775	-2.0362	1.5205
C	2.2792	-3.3701	1.33
C	2.8378	-1.0152	1.6472
C	3.6103	-3.713	1.2693
H	1.5022	-4.1134	1.2106
C	4.1962	-1.3824	1.6036
C	4.5875	-2.6945	1.4232
H	4.9578	-0.6221	1.6988
N	-1.2305	-0.0049	1.6392
N	-0.4201	-2.694	1.4496

O	1.2859	4.3899	1.9329
O	3.7934	3.8005	2.0397
O	5.8757	-3.1154	1.3547
O	4.0911	-4.9595	1.0546
C	3.1314	-5.9879	0.8222
H	3.7093	-6.8953	0.6437
H	2.4878	-6.1321	1.6992
H	2.5162	-5.7588	-0.0563
C	6.896	-2.1441	1.5202
H	6.8529	-1.38	0.7316
H	6.8287	-1.6539	2.5
H	7.84	-2.6854	1.4484
C	5.1903	3.54	2.1068
H	5.547	3.0292	1.2047
H	5.6707	4.5163	2.1747
H	5.4375	2.9462	2.9967
C	-0.0916	4.7478	1.8747
H	-0.5557	4.3737	0.9551
H	-0.6376	4.3594	2.7436
H	-0.1169	5.838	1.8857

dDBP(cis) – lowest energy unfolded conformer with the r2SCAN-3c functional (unfolded in Table S9).

Charge = 0 Multiplicity = 1

C	-2.411	-3.1229	0.5887
C	-3.6115	-2.9645	-0.0673
C	-4.3301	-1.757	0.0501
C	-3.7993	-0.7013	0.8575
C	-2.5673	-0.897	1.5265
C	-1.8878	-2.0771	1.3971
H	-4.0143	-3.7657	-0.6782
H	-2.1861	-0.089	2.1432
H	-0.9548	-2.23	1.9263
C	-5.6124	0.5999	0.3521
C	-6.1493	-0.4647	-0.4569
C	-6.3432	1.8439	0.475
C	-7.5736	2.0102	-0.188
C	-5.8148	2.8848	1.2619
C	-8.2428	3.2397	-0.0341
C	-6.4795	4.0804	1.4029
H	-4.8659	2.7052	1.7496
C	-7.7227	4.2602	0.738
H	-9.1893	3.4	-0.5296
C	-7.4186	-0.2811	-1.1336
C	-8.1199	0.9312	-1.0032
C	-7.9442	-1.3232	-1.9193
C	-9.3487	1.0582	-1.6806
C	-9.1461	-1.1858	-2.5749
H	-7.3666	-2.2355	-1.9871

C	-9.8631	0.0347	-2.4521
H	-9.912	1.9764	-1.6
N	-4.4576	0.4646	0.9901
N	-5.505	-1.6132	-0.5952
C	-1.6991	-4.4164	0.4293
O	-2.1413	-5.3833	-0.1506
O	-0.4845	-4.3877	1.0192
O	-9.7296	-2.1296	-3.3496
O	-11.0324	0.0869	-3.1299
O	-8.3096	5.4635	0.9278
O	-6.0524	5.1355	2.1357
C	-9.0415	-3.366	-3.49
H	-8.0566	-3.224	-3.9529
H	-8.9155	-3.8643	-2.5204
H	-9.6649	-3.9816	-4.139
C	-11.7917	1.2833	-3.0479
H	-12.6782	1.1164	-3.6604
H	-12.0972	1.4935	-2.0143
H	-11.2312	2.1407	-3.4432
C	-9.5539	5.7012	0.287
H	-9.4597	5.6387	-0.8051
H	-10.321	4.9933	0.6275
H	-9.8451	6.7136	0.5681
C	-4.812	4.9893	2.8144
H	-4.647	5.9306	3.3393
H	-4.8486	4.1658	3.539
H	-3.9899	4.8122	2.1092
C	0.3038	-5.5932	0.9671
C	1.0827	-5.6756	-0.3376
C	1.2167	-5.5652	2.187
H	-0.3684	-6.4575	1.0537
C	1.9983	-6.902	-0.328
H	1.6773	-4.7606	-0.4483
H	0.3756	-5.7196	-1.1712
C	2.1522	-6.7662	2.1842
H	0.6177	-5.5206	3.1015
C	2.9388	-6.8805	0.8771
H	2.5709	-6.9444	-1.2609
H	1.3835	-7.8128	-0.295
H	2.8234	-6.6952	3.0468
H	1.5391	-7.666	2.3273
H	3.5574	-7.7846	0.8968
H	3.6241	-6.0279	0.7927
O	2.0337	-4.3708	2.1163
C	1.6617	-3.3055	2.8598
O	0.775	-3.3219	3.6839
C	2.194	-0.9176	3.2807
C	2.8837	0.2365	3.0329
C	3.8914	0.2661	2.0382
C	4.1785	-0.9266	1.3025
C	3.4499	-2.1038	1.5762
C	2.4734	-2.1016	2.5479

H	1.4186	-0.9581	4.0379
H	2.6807	1.1504	3.5823
H	3.6781	-2.9955	1.0037
C	5.7904	0.1828	0.1161
C	5.4968	1.3865	0.853
C	6.8244	0.1976	-0.8993
C	7.5333	1.3825	-1.1684
C	7.1154	-0.9801	-1.6126
C	8.5308	1.3425	-2.1622
C	8.0921	-1.0046	-2.5812
H	6.5414	-1.8641	-1.3686
C	8.8167	0.1857	-2.8602
H	9.0948	2.235	-2.3909
C	6.2312	2.6	0.5632
C	5.9386	3.777	1.2783
C	7.2292	2.6026	-0.4293
C	6.6122	4.9496	1.028
H	5.1634	3.7217	2.0309
C	7.91	3.8106	-0.675
C	7.6209	4.9648	0.0267
H	8.6795	3.8471	-1.4321
N	5.1319	-0.9421	0.3501
N	4.5624	1.4064	1.7944
O	8.442	-2.0858	-3.3161
O	9.76	0.074	-3.8222
O	8.2316	6.1562	-0.1572
O	6.4017	6.1274	1.6601
C	5.3973	6.1502	2.6661
H	5.3808	7.1716	3.0473
H	4.4132	5.8959	2.2523
H	5.6353	5.4567	3.4828
C	9.2457	6.2359	-1.148
H	10.0821	5.5625	-0.9191
H	8.85	6.0003	-2.1446
H	9.5968	7.268	-1.1321
C	10.5201	1.2296	-4.1416
H	11.0863	1.5889	-3.2722
H	11.2144	0.9226	-4.9242
H	9.8801	2.0381	-4.519
C	7.7388	-3.2947	-3.0613
H	7.8812	-3.6275	-2.0252
H	6.6653	-3.1807	-3.2591
H	8.1597	-4.0336	-3.7437

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