

Supplementary Information For
Dielectric-Tuned Charge and Exciton Dynamics in Perylene
Bisimide Supramolecular Aggregates

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Global Analysis

Global analyses of the femtosecond-Transient absorption (fs-TA) spectra were performed using the Glotaran software¹. The procedure evaluates the instrument time response function and the group velocity dispersion of the white continuum and allows one to compute decay time constants and dispersion-compensated spectra. All the wavelengths were analyzed in global analysis concurrently, employing a target model to give evolution-associated difference spectra (EADS) and decay-associated difference spectra (DADS).

Rehm-Weller Analysis

The change in free energy for the charge-separation (ΔG_{CS}) and charge recombination (ΔG_{CR}) were estimated employing the followed relations based on the Born dielectric continuum model².

$$\Delta G_{CS} = e[E_{ox} - E_{red}] - E_{00} + C + S \quad S1$$

$$C = \frac{-e^2}{4\pi\epsilon_0\epsilon_s} \left(\frac{1}{R_{AD}} \right) \quad S2$$

$$S = \frac{e^2}{8\pi\epsilon_0} \left(\frac{1}{r_D} + \frac{1}{r_A} \right) \left(\frac{1}{\epsilon_s} - \frac{1}{\epsilon_{SP}} \right) \quad S3$$

$$\Delta G_{CR} = -(E_{00} + \Delta G_{CS}) \quad S4$$

Where e is the charge of the electron, E_{ox} and E_{red} are the oxidation and first reduction potentials, respectively, ϵ_0 is the permittivity of free space, ϵ_s is the static dielectric constant of the solvent, and ϵ_{SP} is the static dielectric constant of the solvent used for electrochemical measurements, R_{AD} r_A and r_D are the center-to-center distance between the donor (TDOP) and the acceptor (PBI), the ionic radius of the donor, the ionic radius of the acceptor, respectively ($R_{AD} = 8.535 \text{ \AA}$, $r_A = 5.94 \text{ \AA}$, $r_D = 3.4 \text{ \AA}$). The values were estimated from the DFT-optimized geometry under the dimer approximation. E_{00} is the energy of the excited singlet (donor) state. At finite distances, the Coulombic attraction energy (C) between the radical ions is given by a point-charge model as $\left(\frac{1}{\epsilon_s R_{AD}} \right)$.

Driving force charge recombination; The reaction-free energy for charge recombination (CR) was determined to be the difference in free energies between the product ground state (GS) and the reactant charge separation (CS) state.

$$\Delta G_{CR} = E_{CS}(R_{eq}^{CS}) - E_{GS}(R_{eq}^{GS}) \quad S5$$

The first term is the energy calculated at the optimized CS state geometry in the CS redox state using CDFT. While the second term is the energies of the GS at their equilibrium geometries.

Reorganization energy (λ); The total reorganization energy λ is the sum of the inner-sphere (solute) and outer-sphere (solvent) reorganization energies. The reorganization energy for CS and CR were calculated using CDFT for the CS state, and standard DFT for the GS using the ω b97xd functional and the 6-311G(d,p) basis set implemented in Qchem 5.2.2³.

Reorganization energy (λ) was calculated by employing constraint DFT for charge-separated state and DFT for ground-state calculation.

$$\lambda_{CS} = E_{CS}(R_{eq}^{GS}) - E_{CS}(R_{eq}^{CS}) \quad S6$$

The first term is the energy calculated at the optimized GS geometry in the CS redox state. While the second term is the energies of the CS at their equilibrium geometries

$$\lambda_{CR} = E_{GS}(R_{eq}^{CS}) - E_{GS}(R_{eq}^{GS}) \quad S7$$

The first term corresponds to the energy calculated at the optimized CS geometry in the GS state and the second term is the energies of the GS at their equilibrium geometries.

The solvent reorganization energy is computed using the dielectric continuum theory and depends on the radii of the donor (r_D) and acceptor (r_A), the center-to-center distance (R_{DA}), and the optical (ϵ_{op}) and static (ϵ_S) dielectric constants of the solvent as given in eq. S8⁴:

$$\lambda_S = \frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{2r_A} + \frac{1}{2r_D} - \frac{1}{R_{DA}} \right) \left(\frac{1}{\epsilon_{op}} - \frac{1}{\epsilon_S} \right) \quad S8$$

Potential Energy Curve Calculation based on Marcus Theory

The potential energy curves for the locally excited (LE) and charge separated (CS) states were simulated to visualize the driving force (ΔG_{CS}) for the electron transfer (ET) process. The calculations were performed using the interactive module “Marcus Theory of Electron Transfer 3: Interactive Potential Energy Surfaces for Charge Separation” developed by René M. Williams et al., available via the Wolfram Demonstrations Project^{5,6}.

The ET dynamics were analyzed using the classical Marcus theory. The rate of electron transfer (k_{ET}) is described by the following equation,

$$k_{ET} = \sqrt{\frac{\pi}{\hbar^2 \lambda_T k_B T}} V^2 \exp \left[-\frac{(\Delta G_{CS} + \lambda_T)^2}{4 \lambda_T k_B T} \right] \quad S9$$

$\hbar$ is the reduced Planck constant, V is the electronic coupling matrix element between the donor and acceptor units, λ_T is the total reorganization energy (sum of internal, λ_i , and solvent, λ_s , reorganization energies), k_B is the Boltzmann constant and T is the temperature (set to 298 K) and ΔG_{CS} is the Gibbs free energy of CS.

The potential energy curves were modeled as harmonic oscillators (parabolas) along the reaction coordinate, based on the classical Marcus theory of electron transfer. The free energy surfaces for the reactant (excimer like S_1 state) and product (CS state) are described by the following equations,

$$G_{LE}(q) = \lambda_T q^2 \quad S10$$

$$G_{CS}(q) = \lambda_T (q - 1)^2 + \Delta G_{CS} \quad S11$$

where q represents the dimensionless reaction coordinate (0 for the reactant minimum, 1 for the product minimum). To generate the potential energy curves presented in Fig. 4, the input parameters were set to match the computational calculations and the experimental values derived from our spectroscopic and electrochemical measurements (relative energy levels were aligned by first defining S1 and CS energetics and then applying the same procedure to the CR step to establish the ground-state reference). The reorganization energy (λ_T) was estimated to be 0.40, 0.42, 0.64, 0.76 eV and the driving force (ΔG_{CS}) was set to -0.516, -0.639, -0.950, -1.112 eV in MCH, TOL, DEE, THF, respectively. The electronic coupling matrix element (V) was assumed to be diabatic for the qualitative representation of the crossing point.

Theoretical Modeling and Fitting of Charge Separation and Recombination Rates

To elucidate the mechanism of charge separation and recombination dynamics, we analyzed the dependence of the electron transfer rate (k_{ET}) on the thermodynamic driving force ($-\Delta G_{CS}$ or $-\Delta G_{CR}$) using both classical and semiclassical Marcus theories. The fitting procedures were performed using the “Marcus Theory of Electron Transfer 5” interactive module.^{5,7}

First, for the classical Marcus theory fitting, the rate constant is given by:

$$k_{ET} = \frac{2\pi}{\hbar} V^2 \frac{1}{\sqrt{4\pi\lambda_T k_B T}} \exp\left(-\frac{(\Delta G + \lambda_T)^2}{4\lambda_T k_B T}\right) \quad \text{S12}$$

As shown in Fig 4., the classical model adequately reproduces the rate dependence in relatively polar solvent conditions. However, it does not match with the data obtained from relatively low polar solvent conditions.

To account for the discrepancy in the fitting result, we employed the semiclassical Marcus-Levich-Jortner (MLJ) theory.⁸ This model incorporates the coupling of the electron transfer to a quantized

high-frequency vibrational mode (1400 cm⁻¹, C=C stretching mode in this study)⁹, which nuclear tunneling through the activation barrier. The MLJ rate equation is expressed as:

$$k_{ET} = \frac{2\pi}{\hbar} V^2 \frac{1}{\sqrt{4\pi\lambda_S k_B T}} \sum_{n=0}^{\infty} \exp(-S) \frac{S^n}{n!} \exp\left(-\frac{(\Delta G + \lambda_S + n\hbar\omega)^2}{4\lambda_S k_B T}\right) \quad S13$$

where, S is the Huang-Rhys factor ($S = \lambda_v/\hbar\omega$), representing the electron-phonon coupling strength, where λ_v is the vibrational reorganization energy, and n is the vibrational quantum number. The experimental data were fitted to the MLJ equation by optimizing V . The best-fit parameters yielded $V = 80$ meV for CS of all dielectric conditions and $V = 50$ for CR, respectively. The inclusion of the quantized vibrational modes significantly improved the fit in all data from relatively polar solvent to nonpolar solvent condition, confirming that nuclear tunneling plays a critical role in the charge dynamics of the **D-PBI-D_{agg}** in nonpolar regime.

Exciton Diffusion Coefficient and Length Calculation by One-dimensional Exciton Diffusion Model

Here, we describe the one-dimensional (1D) exciton diffusion model used to estimate the exciton diffusion coefficient (D) from the early-time exciton-exciton annihilation (EEA). The procedure consists of converting the experimental pump fluence into the initial excitation density per units (n_0) within the pump-probe overlap volume, extracting an effective bimolecular annihilation rate constant (γ_{eff}) from the EEA time constant (τ_{EEA}), and mapping γ_{eff} onto the 1D diffusion-limited annihilation form to obtain D . We first converted the pump fluence into the initial exciton density by considering the absorbed photon at excitation wavelength ($OD = 1$), the optical path length ($d = 100 \mu m = 0.01 cm$), and the chromophore concentration ($C_{PBI} = 10 mM = 0.01 M$).

$$\langle n^* \rangle_{vol} = \frac{N_{pump}}{\pi r_{probe}^2 d} \left[1 - 10^{-OD(\lambda_{pump})} \right] \quad S14$$

$$N_{pump} = \frac{E_{pump} \lambda_{pump} \int_0^{r_{probe}} r e^{-2r^2/r^2_{pump}} dr}{hc \int_0^{\infty} r e^{-2r^2/r^2_{pump}} dr} \quad S15$$

$$\langle n^* \rangle_{vol} = E_{pump} \cdot (6.2 \times 10^{22} J^{-1} cm^{-3}) \quad S16$$

$$\langle n^* \rangle_{mol} = \frac{E_{pump}}{C_{PBI}} \cdot (6.2 \times 10^{22} J^{-1} cm^{-3}) \quad S17$$

Under the highest pump-fluence condition (670 $\mu J/cm^2$), this procedure yields an average initial exciton density of $n_0 \approx 4.3 \times 10^{-2}$ excitons per PBI unit.¹⁰

The early-time acceleration of the normalized kinetics (Fig. 5) was fitted using a rate equation that includes both monomolecular decay and bimolecular annihilation terms.

$$\frac{dn(t)}{dt} = -\frac{n(t)}{\tau_{S1}} - \gamma(t)n^2(t) \quad S18$$

The intrinsic lifetime of the excimer-like S_1 state was assumed as the CS time constant for each solution, and $\gamma(t)$ is the time-dependent annihilation rate constant. Assuming diffusion-limited annihilation in a one-dimensional PBI column, $\gamma(t)$ can be expressed as, $\gamma_{1D}(t) = \sqrt{2D/(\pi t)}$, where D is the one-dimensional exciton diffusion coefficient along the stack. In the high-density limit where the annihilation term dominates the early-time dynamics, the characteristic annihilation time $\tau_{EEA} \approx 700$ fs extracted from the fluence-dependent traces, which is consistent in all solvent conditions, can be related to the effective rate constant via $\gamma_{eff} \approx 1/n_0 \tau_{EEA}$. Combining γ with the 1D diffusion-limited expression for $\gamma_{1D}(t) = \sqrt{2D/\pi t}$ at $t = \tau_{EEA}$ yields an exciton diffusion coefficient of $D \approx 150 \text{ nm}^2/ps$ along the PBI column. Using this diffusion coefficient, the one-dimensional diffusion length of the excimer-like S_1 exciton is estimated as $L_D = \sqrt{2D\tau_{S1}}$. The diffusion length of S_1 exciton in each solution was calculated as a value of 27.8 nm, 16.7 nm, 25.2 nm, and 76.3 nm in MCH, TOL, DEE, THF, respectively.

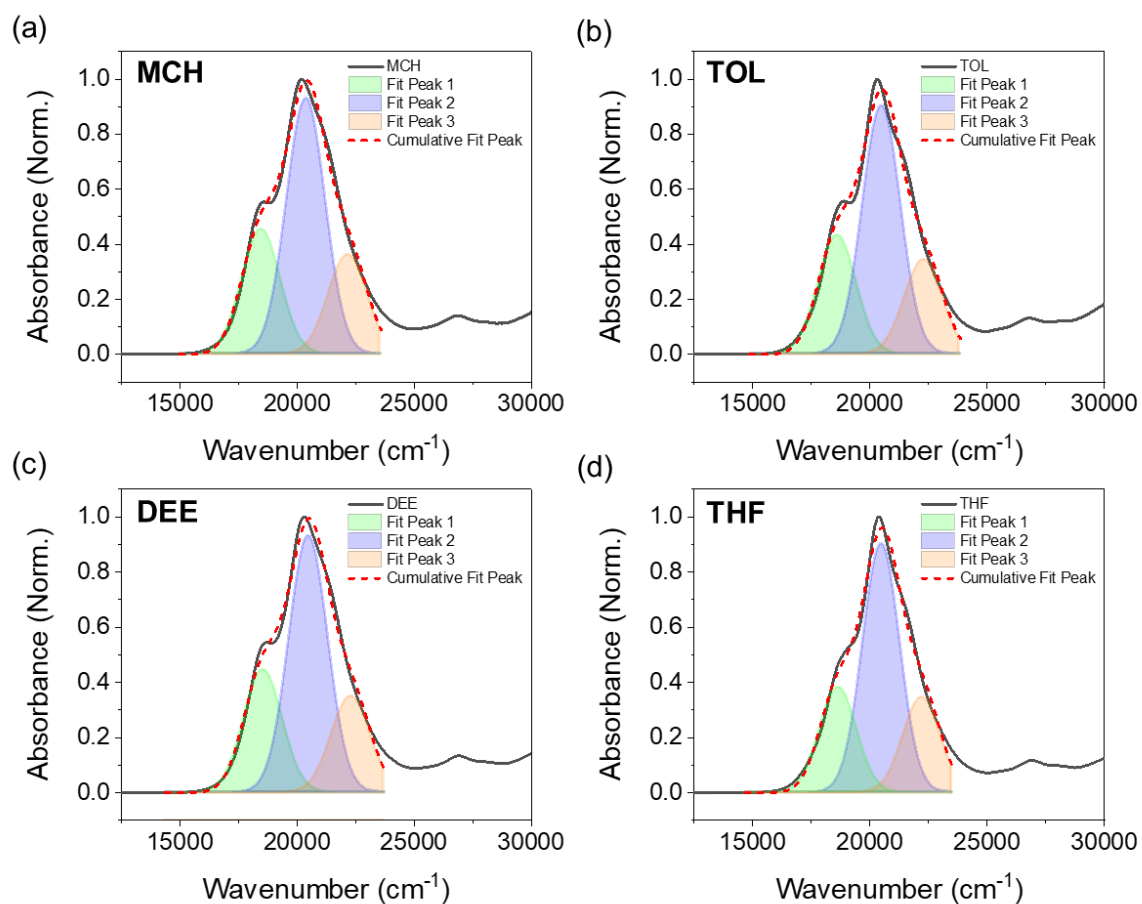


Fig. S1 | The steady-state absorption spectra of **D-PBI-D_{agg}** in (a) methylcyclohexane (MCH), (b) toluene (TOL), (c) diethylether (DEE), and (d) tetrahydrofuran (THF) were fitted using three Gaussian functions.

Table S1 | Gaussian fitting result and calculated coupling constant of absorption spectra of **D-PBI-D_{agg}** in four solvents.

	MCH	TOL	DEE	THF
A_{0-0}/A_{0-1}	0.488	0.479	0.478	0.423
$W (4J_0, \text{cm}^{-1})$	1925	1895	1943	1848
$J_0 (\text{cm}^{-1})$	481	474	486	462

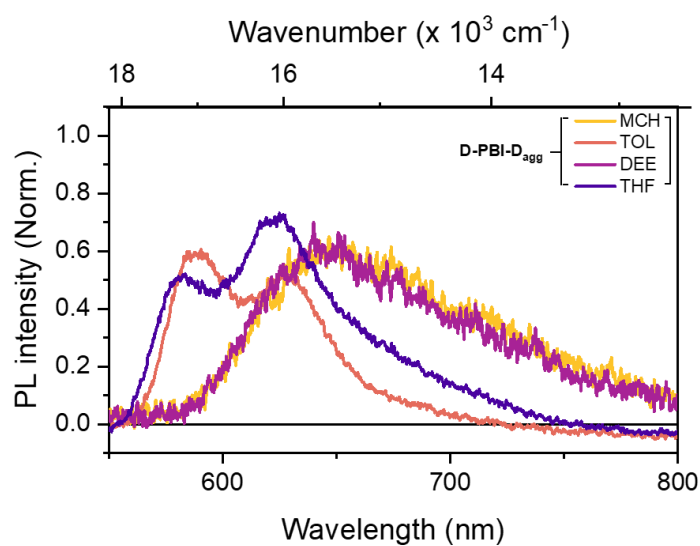


Fig. S2 | The steady-state photoluminescence spectra of **D-PBI-D_{agg}** in all solvents.

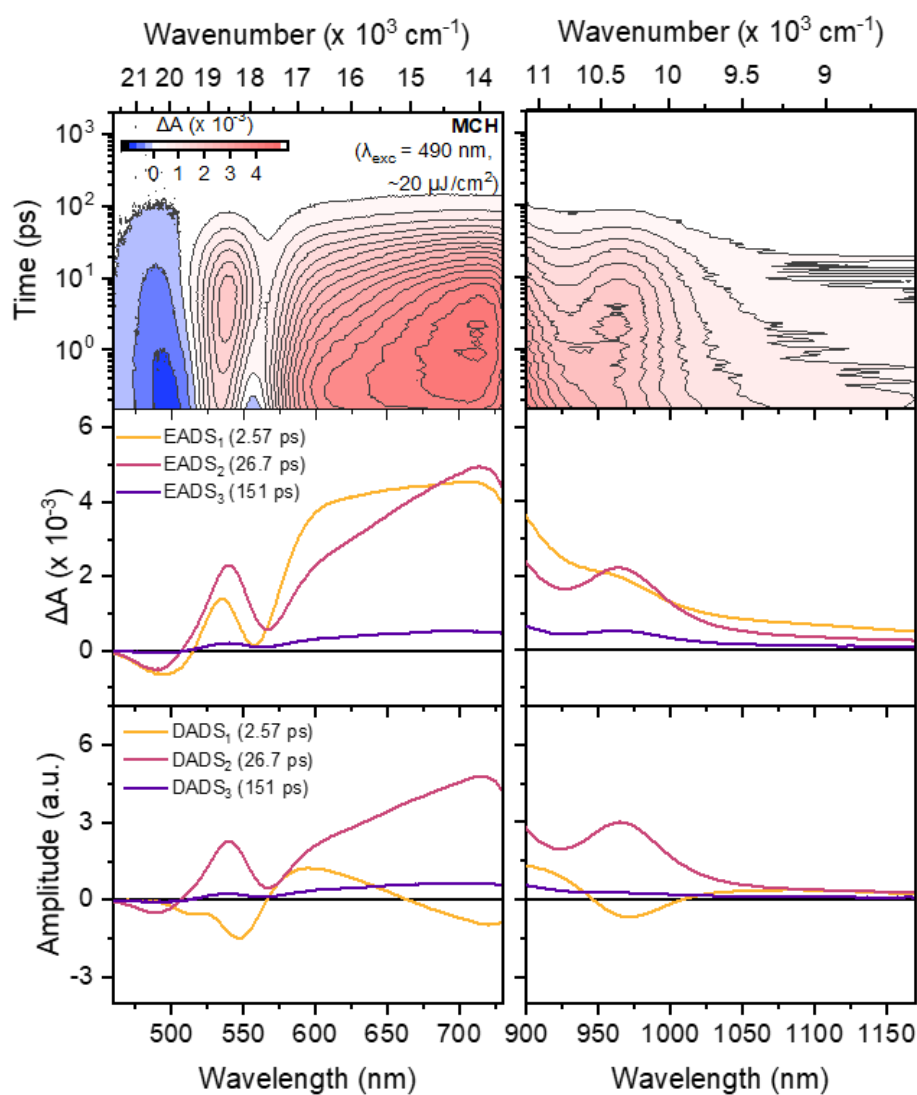


Fig. S3 | Femtosecond transient absorption results in MCH at room temperature. TA contour map (top), evolution-associated difference spectra (EADS, middle), and decay-associated difference spectra (DADS, bottom) of **D-PBI-D_{agg}**. The left and right panels indicate TA results obtained in the visible (460–730 nm) and near-infrared (900–1175 nm) region, respectively. The excitation wavelength was 490 nm with a fluence of $\sim 20 \mu\text{J}/\text{cm}^2$ to avoid EEA.

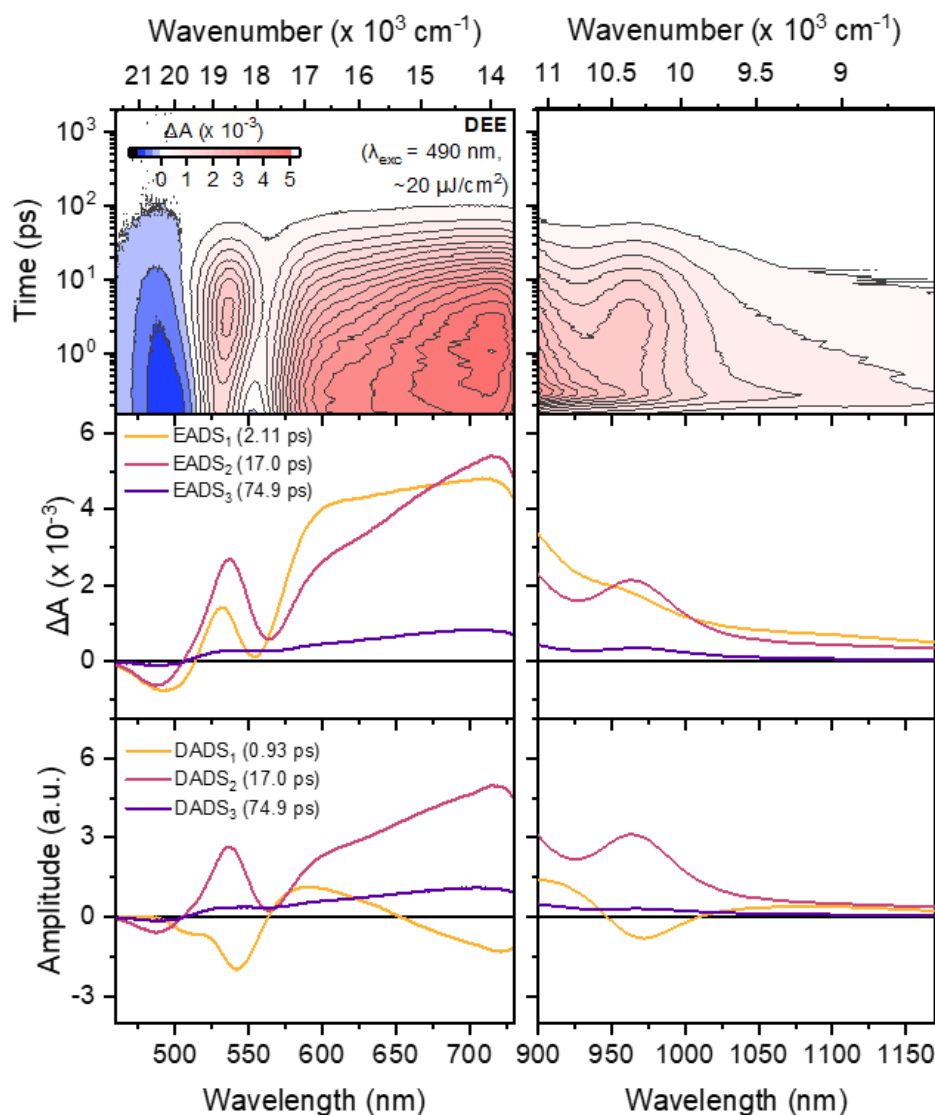


Fig. S4 | Femtosecond transient absorption results in DEE at room temperature. TA contour map (top), evolution-associated difference spectra (EADS, middle), and decay-associated difference spectra (DADS, bottom) of **D-PBI-D_{agg}**. The left and right panels indicate TA results obtained in the visible (460–730 nm) and near-infrared (900–1175 nm) region, respectively. The excitation wavelength was 490 nm with a fluence of $\sim 20 \mu\text{J}/\text{cm}^2$ to avoid EEA.

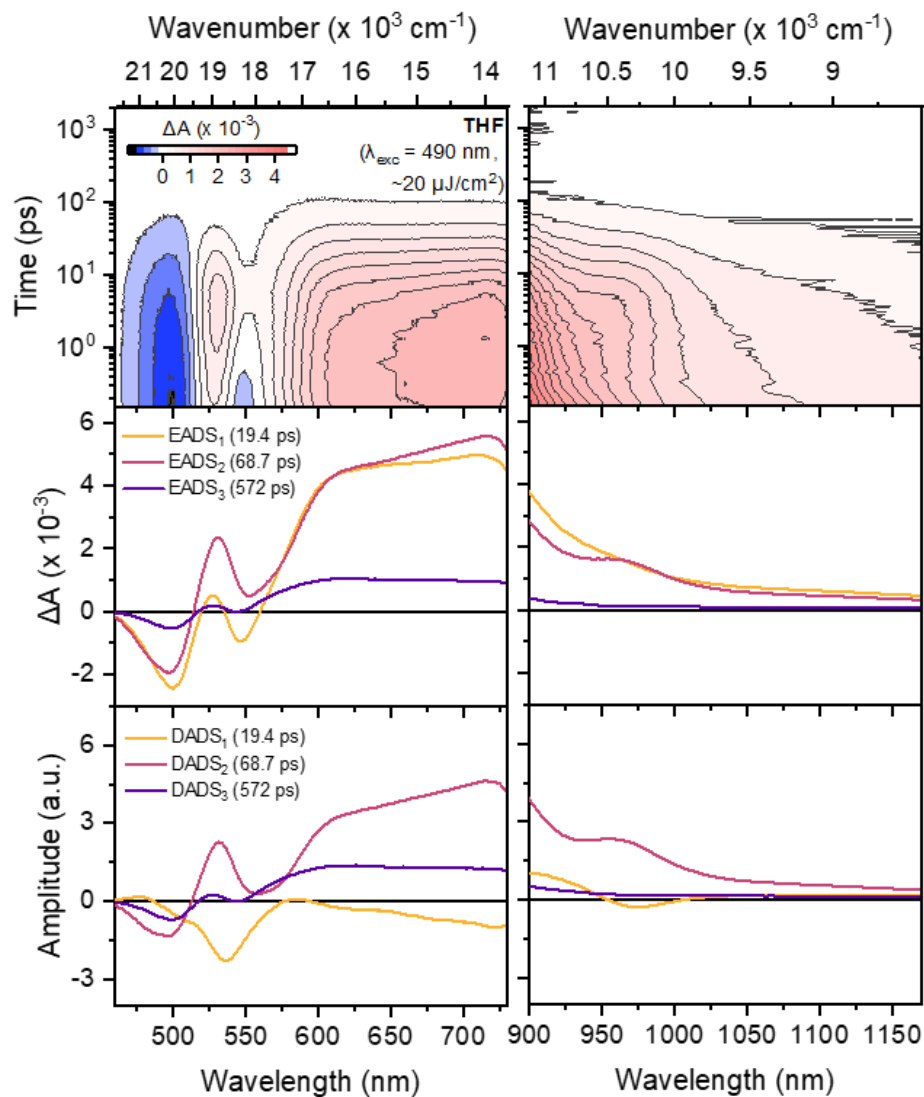


Fig. S5 | Femtosecond transient absorption results in THF at room temperature. TA contour map (top), evolution-associated difference spectra (EADS, middle), and decay-associated difference spectra (DADS, bottom) of **D-PBI-D_{agg}**. The left and right panels indicate TA results obtained in the visible (460–730 nm) and near-infrared (900–1175 nm) region, respectively. The excitation wavelength was 490 nm with a fluence of ~ 20 μJ/cm² to avoid EEA.

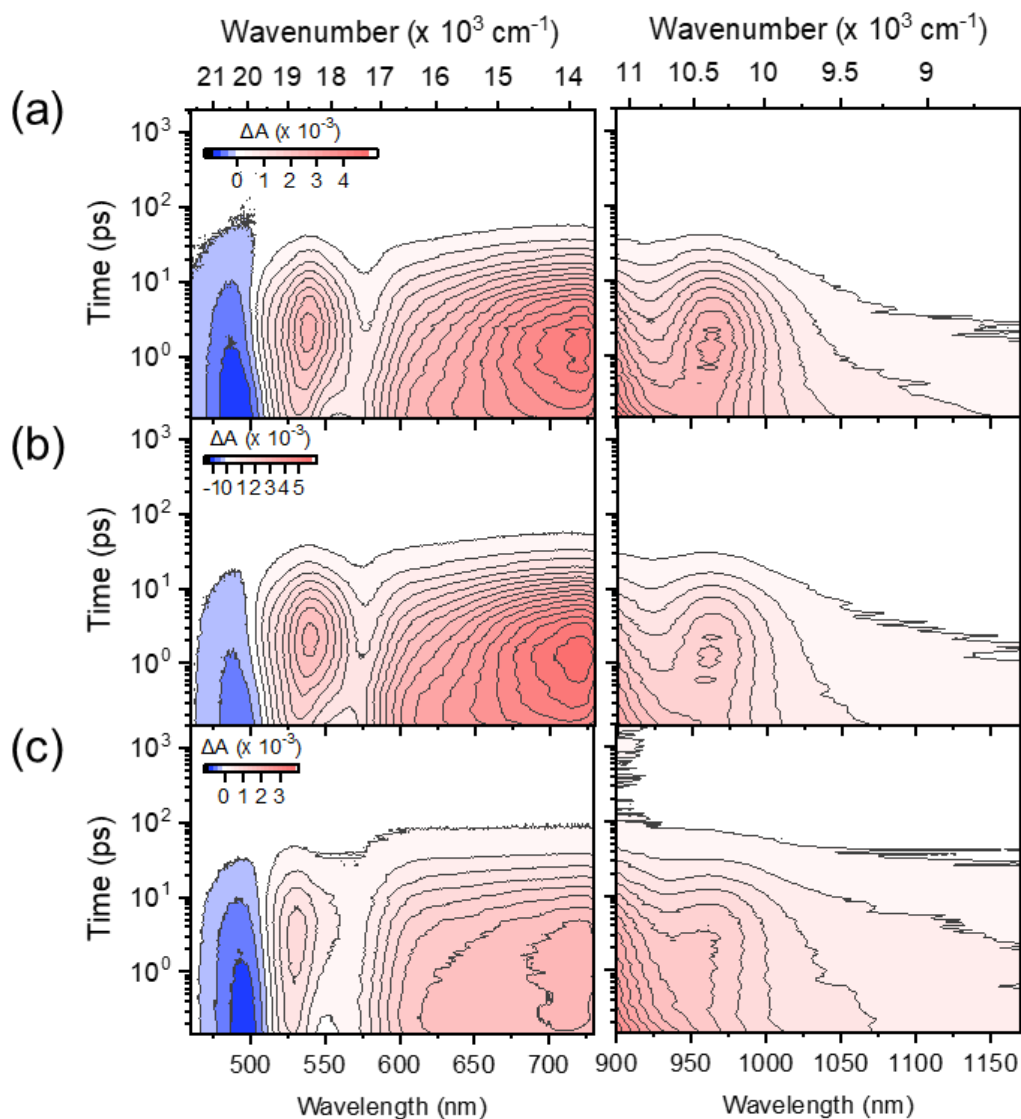


Fig. S6 | Femtosecond transient absorption spectra of **D-PBI-D_{agg}** in the mixed solvents: (a) MCH/TOL ($v:v = 1:1$), (b) TOL/DEE ($v:v = 1:1$), and (c) DEE/THF ($v:v = 1:1$) at room temperature. TA spectra were recorded in the visible (460–730 nm) and near-infrared (900–1175 nm) region. The excitation wavelength was 490 nm with a fluence of $\sim 20 \mu\text{J}/\text{cm}^2$ to avoid EEA.

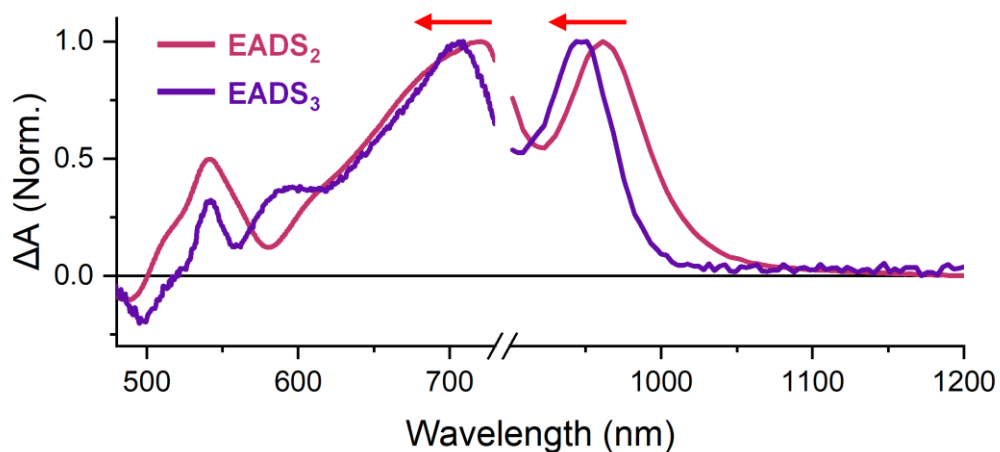


Fig. S7 | EADS₂ and EADS₃ of **D-PBI-D_{agg}** in TOL obtain from global analysis. Blue-shifted spectrum of EADS₃ shows the feature of localized radical anion compared to EADS₂.

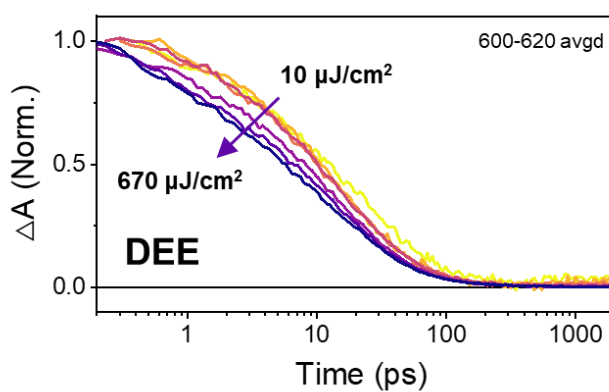


Fig. S8 | Pump-fluence dependence of transient absorption kinetics. Normalized by dividing max value from kinetic profiles of the TA signal averaged from 600–620 nm in DEE. The fluence applied to **D-PBI-D_{agg}** is between 10 and 670 $\mu\text{J}/\text{cm}^2$

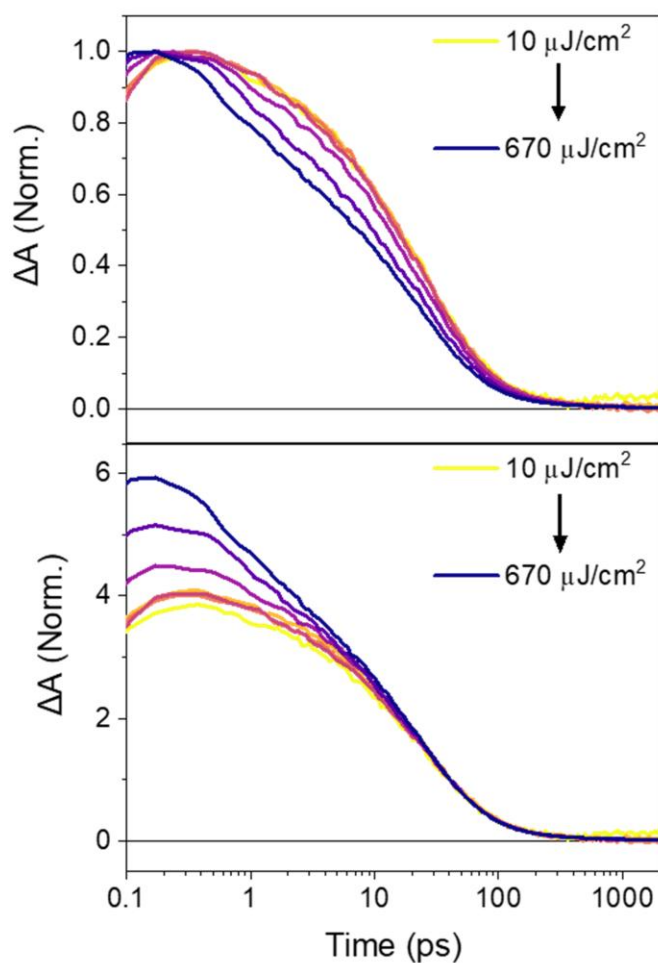


Fig. S9 | Pump-fluence dependence of transient absorption kinetics. Normalized by dividing max value from kinetic profiles of the TA signal averaged from 600-620 nm in MCH (upper panel). Normalized by 40 ps signal value from kinetic profiles of the TA signal averaged from 600-620 nm in MCH (lower panel). The fluence applied to **D-PBI-D_{agg}** is between 10 and 670 μJ/cm².

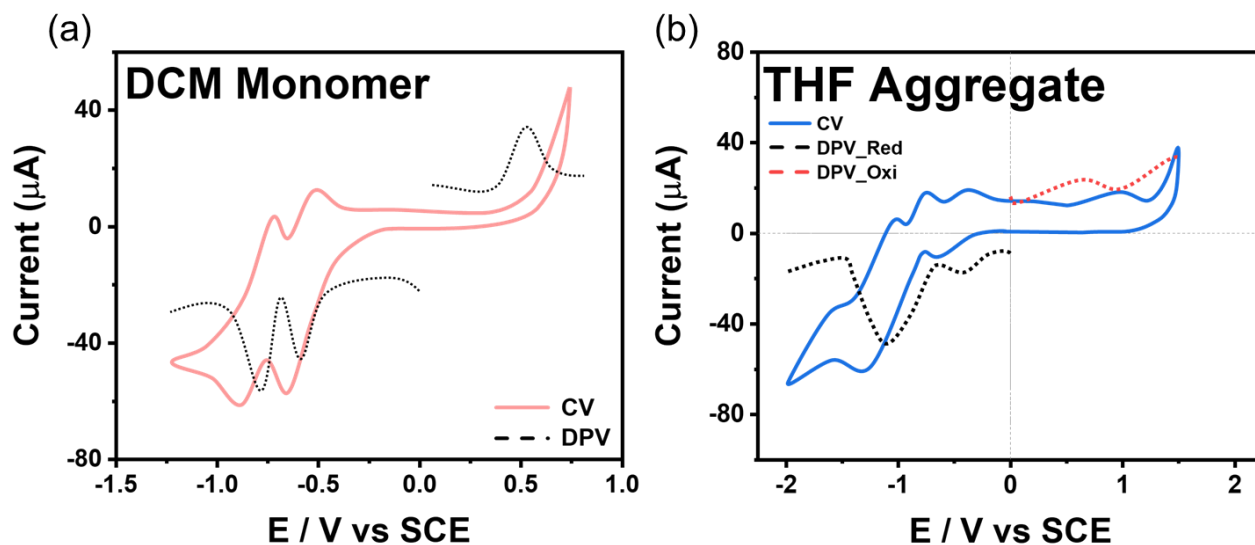


Fig. S10 | Cyclic voltammetry (CV) data and differential pulse voltammetry (DPV) of (a) **D-PBI-D** in Dichloromethane (Tetrabutylammonium perchlorate, TBAP (1 mM) as supporting electrolyte, scan rate 100 mVs⁻¹) and (b) **D-PBI-D_{agg}** in THF (TBAP (0.1 M) as supporting electrolyte, scan rate 100 mVs⁻¹)

Table S2 | Summary of redox potentials (vs SCE) of **D-PBI-D** and **D-PBI-D_{agg}**

	$E_{ox}(D)^1$	$E_{red}(A)^2$	$E_{red}(A)^3$
D-PBI-D	0.52 V	-0.58 V	-0.78 V
D-PBI-D_{agg}	0.82 V	-0.39 V	-1.10 V

¹Irreversible, ²first reduction of D-PBI-D and D-PBI-D_{agg}, ³ second reduction of D-PBI-D and D-PBI-D_{agg}

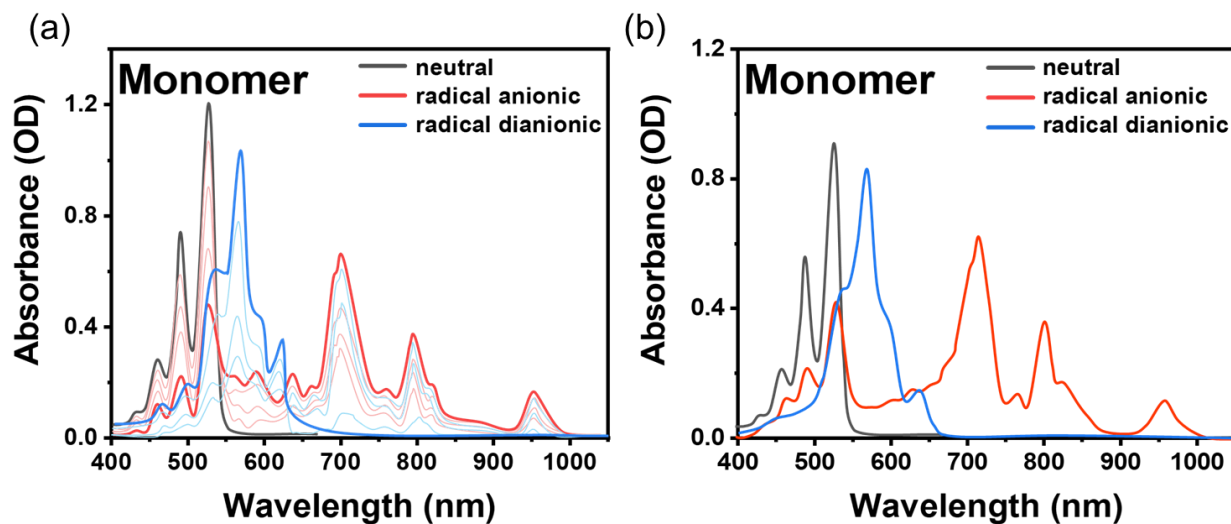


Fig. S11 | (a) Spectroelectrochemistry spectra of **D-PBI-D** in DCM with TBAP (1 mM) and (b) upon addition of $\text{Na}_2\text{S}_2\text{O}_4$ (10 mM).

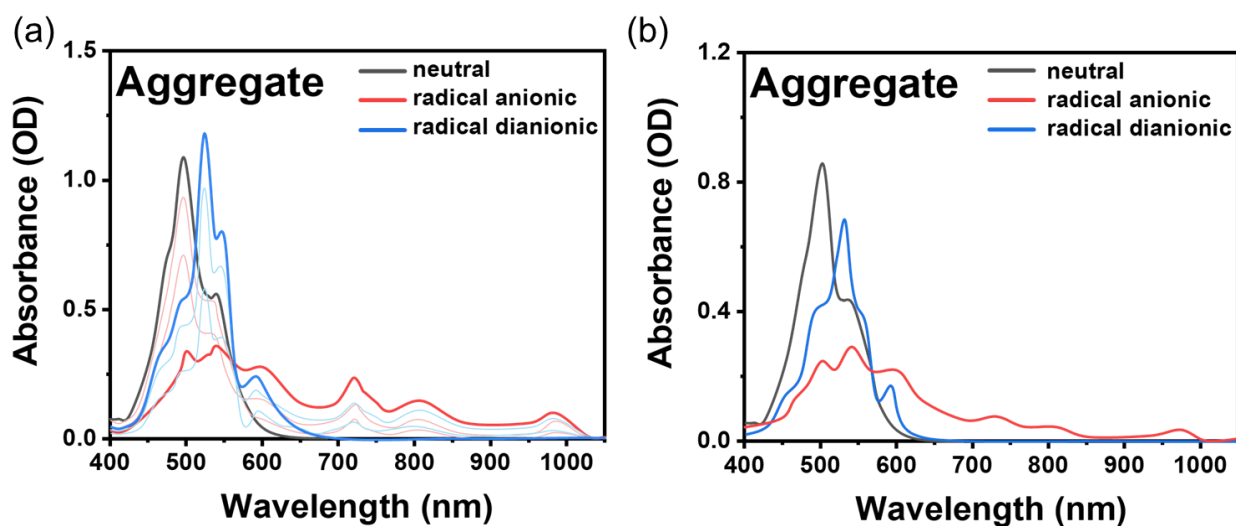


Fig. S12 | (a) Spectroelectrochemistry spectra of **D-PBI-D_{agg}** in THF with TBAP (0.1 M) and (b) upon addition of Na_2SO_3 (10 mM).

Table S3 | ΔG_{CS}^1 and ΔG_{CR}^2 values of **D-PBI-D_{agg}** in various polar solvents.

	MCH	MCH+ TOL ³	TOL	TOL+ DEE ³	DEE	DEE+ THF ³	THF
ΔG_{CS} (eV)	-0.516	-0.583	-0.639	-0.840	-0.950	-1.053	-1.112
ΔG_{CR} (eV)	-1.584	-1.517	-1.461	-1.260	-1.150	-1.047	-0.988

¹Calculated using eq.S1, ²Calculated using eq.S4, ³For mixed solvent: average of both values.¹¹**Table S4** | Computed reorganization energies of CS and CR of **D-PBI-D_{agg}** by employing CDFT and DFT.

	Solvent	λ_{CS} (eV)	λ_{CR} (eV)	λ_s^1	$\lambda_{i(CS)}^2$ (eV)	$\lambda_{i(CR)}^3$ (eV)
D-PBI-D_{agg}	MCH	0.40	0.67	0	0.40	0.67
	TOL	0.42	0.766	0.043	0.377	0.723
	DEE	0.64	1.505	0.520	0.12	0.985
	THF	0.76	1.659	0.615	0.145	1.044

¹Calculated using eq.S8, ²inner-sphere reorganization energy for CS state ($\lambda_{CS} = \lambda_{i(CS)} + \lambda_s$), ³inner-sphere reorganization energy for CR state ($\lambda_{CR} = \lambda_{i(CR)} + \lambda_s$).**Table S5** | Distances and torsional angles between the two monomers of **D-PBI-D_{agg}** in various solvents for the GS state.

	Dimer Distance ¹	Dimer Torsional angle ²
MCH	3.3932 Å	106.530°
TOL	3.3945 Å	107.087°
DEE	3.3968 Å	110.706°
THF	3.3972 Å	113.479°

¹Distance between PBI-PBI cores in the dimer, ²Torsion angle referenced to the nitrogen atom of PBI in the dimer.

Table S6 | Cartesian coordinates for optimized ground state and CS state geometries for **D-PBI-D** dimer in MCH.

Ground state/MCH					CS state/MCH				
No.	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	N	5.521703002	1.741793763	1.268565032	1	N	5.520836165	1.199454578	1.78037281
2	N	-5.538301823	1.65941767	-1.342187602	2	N	-5.537960513	2.034461624	-0.734290449
3	O	4.993913653	1.567158694	3.474448592	3	O	4.984859072	0.244088207	3.776077151
4	O	5.991376102	2.010046187	-0.94106276	4	O	5.997871586	2.207739495	-0.202544008
5	O	-6.034894157	1.965218463	0.852508761	5	O	-6.03854132	1.523934174	1.425174174
6	O	-5.008664038	1.371127806	-3.534772799	6	O	-4.988019989	2.53230993	-2.885798406
7	C	3.721004737	1.729476308	-0.393147092	7	C	3.723838524	1.770359014	0.212750156
8	C	3.332043683	1.701792995	-1.708323487	8	C	3.337437671	2.23489699	-1.018140239
9	C	1.97550347	1.639691028	-2.038199677	9	C	1.981156145	2.303995073	-1.348245349
10	C	0.991366621	1.635664997	-1.068391838	10	C	0.994348412	1.93785589	-0.453380401
11	C	-0.439840695	1.591316713	-1.410761966	11	C	-0.435970707	2.021837884	-0.79094884
12	C	-0.88207599	1.500346365	-2.718986225	12	C	-0.875789424	2.424954018	-2.039726727
13	C	-2.243420399	1.46554055	-3.032676751	13	C	-2.235834976	2.499004688	-2.35105795
14	C	-3.186777363	1.534364221	-2.036794611	14	C	-3.181069742	2.184226917	-1.406311319
15	C	-2.779011713	1.632241386	-0.691264398	15	C	-2.777197657	1.782889598	-0.118004009
16	C	-3.748873877	1.722607153	0.328103689	16	C	-3.752614764	1.479101722	0.853895861
17	C	-3.359616885	1.788313328	1.642184142	17	C	-3.367865258	1.042175943	2.096027464
18	C	-2.002530229	1.765590511	1.976621846	18	C	-2.010682705	0.900415306	2.403178271
19	C	-1.016632412	1.69987871	1.010697555	19	C	-1.019715861	1.21503799	1.492933132
20	C	-1.400594424	1.641042349	-0.362041792	20	C	-1.399773713	1.673202607	0.196542779
21	C	1.375345852	1.673720221	0.30437574	21	C	1.375429864	1.464306768	0.836412627
22	C	0.415603026	1.689481935	1.355242688	22	C	0.412545395	1.085171629	1.81395964
23	C	0.862144282	1.691191197	2.665180088	23	C	0.858595197	0.604625687	3.032604041
24	C	2.22555284	1.675497526	2.977714343	24	C	2.221308673	0.487028971	3.325248193
25	C	3.167342891	1.677750826	1.977958675	25	C	3.165212959	0.862202514	2.401423015
26	C	2.753750791	1.694788052	0.630919698	26	C	2.753510359	1.364205935	1.151097579
27	C	4.610639854	1.651229655	2.332430841	27	C	4.609708042	0.724564205	2.735204045
28	C	5.161651244	1.841503274	-0.074848641	28	C	5.166299602	1.755640267	0.550121072
29	C	-5.19033605	1.79460217	0.002057267	29	C	-5.195571789	1.669065615	0.571082932
30	C	-4.625736579	1.502891023	-2.396118891	30	C	-4.619395254	2.264259003	-1.768135053
31	H	4.087703411	1.727110123	-2.483636828	31	H	4.097438708	2.547160231	-1.723908964
32	H	1.715576093	1.602030738	-3.08677425	32	H	1.723347275	2.665827608	-2.333847303
33	H	-0.175350947	1.451037176	-3.535723607	33	H	-0.165787772	2.691624998	-2.810534617
34	H	-2.571080502	1.386705596	-4.062053573	34	H	-2.565433469	2.80344505	-3.337117625
35	H	-4.11609045	1.859060807	2.414163202	35	H	-4.129636891	0.805224498	2.829099568

36	H	-1.743624337	1.809234096	3.025398585	36	H	-1.755067102	0.537258858	3.388873865
37	H	0.157900106	1.69734571	3.485847759	37	H	0.150784768	0.301492207	3.792194949
38	H	2.55460126	1.66022543	4.009633224	38	H	2.552347701	0.10063916	4.281707797
39	N	5.527449758	-1.70817672	-1.044012788	39	N	5.512992825	-1.180410294	-1.724558028
40	N	-5.612969807	-1.697932383	1.200305449	40	N	-5.563348447	-2.038339259	0.687288951
41	O	5.933016494	-1.935279123	1.181749344	41	O	5.97880834	-2.164918232	0.27234837
42	O	5.074801695	-1.556290901	-3.267248158	42	O	4.995087873	-0.248040331	-3.735797678
43	O	-5.154424551	-1.409319623	3.40950909	43	O	-5.031204264	-2.578213655	2.833132354
44	O	-6.029029391	-2.031005891	-1.007984644	44	O	-6.045399884	-1.508420622	-1.471297729
45	C	3.200092982	-1.667151541	-1.829306505	45	C	3.164062344	-0.870131717	-2.376319576
46	C	2.291449095	-1.671202762	-2.859497634	46	C	2.227325675	-0.501356416	-3.310158766
47	C	0.918995193	-1.694995079	-2.592028182	47	C	0.862798853	-0.624232763	-3.030242613
48	C	0.42971289	-1.698964748	-1.297392696	48	C	0.407488372	-1.10537095	-1.815106661
49	C	-1.013043546	-1.719915845	-1.000189107	49	C	-1.026988507	-1.236110109	-1.505904987
50	C	-1.965791347	-1.793641989	-1.998239946	50	C	-2.010059453	-0.919837747	-2.423867338
51	C	-3.333208747	-1.826173522	-1.708639548	51	C	-3.369700845	-1.056655924	-2.125992341
52	C	-3.766167176	-1.761352402	-0.408308224	52	C	-3.7638989	-1.493186001	-0.886925206
53	C	-2.830936845	-1.662587539	0.64219647	53	C	-2.796834635	-1.8025011	0.091312429
54	C	-3.284605333	-1.563015601	1.972347799	54	C	-3.211614289	-2.206991923	1.375135315
55	C	-2.375345167	-1.487501366	2.998948141	55	C	-2.274448665	-2.526895115	2.325963096
56	C	-1.00387442	-1.516553714	2.731102613	56	C	-0.911852601	-2.451926495	2.025811192
57	C	-0.517569662	-1.606647421	1.438768536	57	C	-0.461911375	-2.045069289	0.781950669
58	C	-1.442503063	-1.662946691	0.35874743	58	C	-1.417290207	-1.694794827	-0.21283255
59	C	1.353957917	-1.676681662	-0.215375596	59	C	1.362288625	-1.48133637	-0.828698073
60	C	0.924318871	-1.641621314	1.143732824	60	C	0.970869475	-1.95665833	0.457535003
61	C	1.875183166	-1.637309659	2.14615454	61	C	1.949949006	-2.317097075	1.363145658
62	C	3.242326551	-1.684413945	1.861898686	62	C	3.308835045	-2.236947881	1.048648312
63	C	3.674969374	-1.707804379	0.56011579	63	C	3.704270088	-1.770866278	-0.178906589
64	C	2.742925164	-1.685065677	-0.496400377	64	C	2.742747123	-1.373119427	-1.129372099
65	C	5.125689247	-1.795015697	0.29099843	65	C	5.148784417	-1.734299135	-0.494437771
66	C	4.652913803	-1.634173821	-2.13747652	66	C	4.609773276	-0.723224801	-2.695941544
67	C	-4.735935358	-1.539408995	2.283676032	67	C	-4.653484761	-2.290715241	1.724121266
68	C	-5.217155814	-1.843977708	-0.129014954	68	C	-5.209628239	-1.670381784	-0.611569039
69	H	2.654087562	-1.654299204	-3.880010389	69	H	2.565592389	-0.114614605	-4.263928346
70	H	0.241827338	-1.704011701	-3.435165614	70	H	0.160901347	-0.324088473	-3.796367142
71	H	-1.671446046	-1.83661562	-3.037636946	71	H	-1.746325314	-0.556268515	-3.407242855
72	H	-4.063113708	-1.903656312	-2.505021901	72	H	-4.126268108	-0.814038566	-2.862531916
73	H	-2.737889283	-1.408751135	4.016538022	73	H	-2.612371582	-2.835675936	3.307825217
74	H	-0.324814974	-1.461281414	3.57080813	74	H	-0.208316908	-2.721244838	2.801582488
75	H	1.579202293	-1.602992027	3.18524068	75	H	1.683844648	-2.679171569	2.346363962
76	H	3.972268699	-1.698002711	2.661883874	76	H	4.064337058	-2.538000766	1.764132542

77	C	-6.940454587	1.762126686	-1.671276552	77	C	-6.936573492	2.240781694	-1.025916537
78	C	-7.459389934	3.024631252	-1.933134342	78	C	-7.412521088	3.546457327	-1.053244019
79	C	-7.724404401	0.629069062	-1.70064624	79	C	-7.757628544	1.160186499	-1.265358636
80	C	-8.811329616	3.149703268	-2.227449714	80	C	-8.752052388	3.775738448	-1.339513562
81	C	-9.081710473	0.761087828	-1.974915128	81	C	-9.102636023	1.394705127	-1.531815084
82	C	-9.638320273	2.010717068	-2.225949621	82	C	-9.608544188	2.689788275	-1.583582995
83	O	-9.427311784	4.316408577	-2.526679778	83	O	-9.327698617	4.999556084	-1.399632105
84	O	-10.9643101	2.097914439	-2.524479406	84	O	-10.91590287	2.893537591	-1.909375151
85	O	-9.868741486	-0.35156947	-1.944409452	85	O	-9.936677299	0.32744694	-1.700570196
86	C	-8.675796385	5.510413563	-2.417961893	86	C	-8.500777093	6.127685513	-1.215486391
87	C	-10.34039119	-0.78759991	-3.214774607	87	C	-10.3490612	0.094704581	-3.041125134
88	C	-11.75093489	2.945127533	-1.684700868	88	C	-11.7547498	3.201940409	-0.80463294
89	H	-6.80411978	3.8839081	-1.903889143	89	H	-6.730153068	4.362380634	-0.86032295
90	H	-7.311212452	-0.353364679	-1.517967976	90	H	-7.392599748	0.141703907	-1.242367714
91	H	-9.369124507	6.320026094	-2.636071977	91	H	-9.148406927	6.994664472	-1.331000311
92	H	-7.854712167	5.531353168	-3.142360212	92	H	-7.70684955	6.164637779	-1.969643898
93	H	-8.274977518	5.635474228	-1.406511762	93	H	-8.055216652	6.141250442	-0.214106829
94	H	-10.9169323	-1.693162622	-3.031664235	94	H	-10.98542409	-0.788956262	-3.015464674
95	H	-9.498361942	-1.018588846	-3.875751886	95	H	-9.479996574	-0.101332917	-3.678133627
96	H	-10.97814045	-0.030073959	-3.676633879	96	H	-10.91408504	0.945785404	-3.429481533
97	H	-12.72976691	2.473593162	-1.585201568	97	H	-12.76431538	3.296664422	-1.202980499
98	H	-11.85583284	3.931935554	-2.140561948	98	H	-11.45690832	4.145441367	-0.3385327
99	H	-11.29519451	3.048992293	-0.698738319	99	H	-11.72840726	2.396775976	-0.063762308
100	C	-7.024676211	-1.811957055	1.490814869	100	C	-6.965391014	-2.250272746	0.965818744
101	C	-7.810358251	-0.680809862	1.532931766	101	C	-7.740973337	-1.211351118	1.42984108
102	C	-7.542830301	-3.084166923	1.701988066	102	C	-7.483173733	-3.521399577	0.746627298
103	C	-9.169352851	-0.815201492	1.811972911	103	C	-9.087986092	-1.449993206	1.696829349
104	C	-8.896837192	-3.217309002	1.983359127	104	C	-8.822802271	-3.760011173	1.024110265
105	C	-9.71537624	-2.076257228	2.04453059	105	C	-9.632359256	-2.717952387	1.50518646
106	O	-9.908627439	0.322467348	1.912903638	106	O	-9.825438867	-0.428224128	2.210355744
107	O	-11.03859747	-2.234303948	2.344583711	107	O	-10.9428777	-2.977702183	1.784520021
108	O	-9.516164901	-4.391630794	2.235437556	108	O	-9.434321469	-4.958393476	0.889615806
109	C	-11.33479441	-1.975168576	3.712868366	109	C	-11.19729752	-3.140033883	3.173663947
110	C	-11.08764457	0.411937762	1.11055091	110	C	-10.98506996	-0.04290442	1.473270649
111	C	-8.741768839	-5.572508797	2.170974245	111	C	-8.667951034	-6.037075533	0.404575689
112	H	-7.393216693	0.299572673	1.348058874	112	H	-7.335818483	-0.220383691	1.587838359
113	H	-6.885006675	-3.940357113	1.6516781	113	H	-6.830802316	-4.300580784	0.378158889
114	H	-12.3974166	-2.175878909	3.845587303	114	H	-12.25705428	-3.374931755	3.270505926
115	H	-11.12078023	-0.931451403	3.966006082	115	H	-10.97009262	-2.219127884	3.7210047
116	H	-10.75439305	-2.636692536	4.363717318	116	H	-10.60421449	-3.965110587	3.581431749
117	H	-11.33383572	1.471957619	1.071747018	117	H	-11.27230028	0.931268069	1.869738136

118	H	-11.91823224	-0.142331393	1.5505188	118	H	-11.80095603	-0.755906773	1.610981637
119	H	-10.89231185	0.042816162	0.100685907	119	H	-10.75385354	0.0414926	0.408063718
120	H	-9.428400554	-6.389659557	2.382731251	120	H	-9.344766639	-6.888481737	0.363577464
121	H	-7.94152222	-5.568063224	2.919405771	121	H	-7.832498138	-6.272249361	1.074505652
122	H	-8.308646484	-5.71014732	1.174376821	122	H	-8.280631645	-5.834516928	-0.600643937
123	C	6.930271108	1.824975199	1.582066909	123	C	6.929408105	1.180159456	2.105233788
124	C	7.498680936	3.08216844	1.729291495	124	C	7.457583433	2.269735405	2.787814948
125	C	7.680928163	0.674634104	1.688781246	125	C	7.71104253	0.12744047	1.686573718
126	C	8.858829019	3.184644171	1.995261093	126	C	8.817793889	2.290015991	3.06790102
127	C	9.046525964	0.775866228	1.935855899	127	C	9.079605546	0.159076817	1.949390466
128	C	9.651499549	2.027625003	2.091726556	128	C	9.637289849	1.231473699	2.641961635
129	O	9.497012448	4.36352646	2.210222731	129	O	9.446606219	3.271465613	3.754740938
130	O	10.97430368	2.049031362	2.398831521	130	O	10.97315594	1.276669574	2.91995133
131	O	9.737702139	-0.383103786	2.064778715	131	O	9.819678017	-0.906251054	1.547229643
132	C	11.84015723	2.846097603	1.601289471	132	C	11.33928572	0.478021333	4.035445914
133	C	10.94203141	-0.538679864	1.316494678	133	C	10.97215427	-0.639319863	0.747442788
134	C	8.748123595	5.556810881	2.105606162	134	C	8.66908378	4.352605618	4.215628788
135	H	6.876536306	3.961512083	1.641078262	135	H	6.802138991	3.074755621	3.088572765
136	H	7.25259105	-0.309241861	1.556968025	136	H	7.302317143	-0.715001594	1.145283233
137	H	12.84071616	2.438505495	1.747178824	137	H	12.41136049	0.614093383	4.177647052
138	H	11.81037841	3.890521514	1.909173057	138	H	11.1232223	-0.579687894	3.847990762
139	H	11.57104757	2.77017283	0.541457858	139	H	10.81088789	0.804930718	4.93711129
140	H	11.00479419	-1.593672304	1.047994601	140	H	11.11222537	-1.512194247	0.110755005
141	H	11.80840116	-0.25389354	1.916216343	141	H	11.85707519	-0.479961565	1.367749922
142	H	10.90884869	0.054064556	0.399777714	142	H	10.80556	0.237578553	0.118592837
143	H	9.449627495	6.365883643	2.300131183	143	H	9.357359986	5.012458836	4.740734717
144	H	7.943526985	5.590477668	2.847916747	144	H	7.887211429	4.018401692	4.907722818
145	H	8.32498229	5.676202295	1.102213673	145	H	8.209737821	4.901020304	3.385056193
146	C	11.56113138	-2.617383498	-3.00151305	146	C	11.54616806	-1.401178321	-3.882847768
147	C	8.871154421	-5.501768514	-1.334755621	147	C	8.928536814	-4.653021836	-3.109168711
148	C	6.946384888	-1.787539837	-1.305325086	148	C	6.925613607	-1.14463636	-2.02199779
149	C	7.684662111	-0.635791276	-1.440874669	149	C	7.639536941	0.01182331	-1.817841963
150	C	7.53131584	-3.046621351	-1.372817805	150	C	7.532208507	-2.314946468	-2.462493352
151	C	9.059262275	-0.728367418	-1.660102691	151	C	9.013017859	0.015476452	-2.063774835
152	C	8.902793007	-3.13905383	-1.559565805	152	C	8.902277051	-2.321917382	-2.671987444
153	C	9.682107643	-1.974662488	-1.711434724	153	C	9.657917578	-1.150037269	-2.478565814
154	O	9.727771981	0.451370057	-1.735034079	154	O	9.659535621	1.176878749	-1.790074723
155	O	11.04261283	-2.04777559	-1.802528299	155	O	11.01893726	-1.170224265	-2.58264002
156	O	9.589531924	-4.306102602	-1.57039474	156	O	9.61167176	-3.420759067	-3.028655492
157	C	10.74553237	0.606142319	-2.715143476	157	C	10.66723749	1.635891867	-2.677214782
158	H	12.64228034	-2.489770145	-2.955789945	158	H	12.62424361	-1.263380783	-3.802508826

159	H	11.16885684	-2.090680302	-3.878317315	159	H	11.13897241	-0.678147708	-4.598770482
160	H	11.31795879	-3.678209357	-3.072342439	160	H	11.32848037	-2.414342502	-4.223598381
161	H	9.608687543	-6.301531506	-1.354667585	161	H	9.683325253	-5.397703458	-3.354886729
162	H	8.123240527	-5.678860403	-2.114869535	162	H	8.167087146	-4.639878276	-3.897228977
163	H	8.381975305	-5.482725754	-0.355380072	163	H	8.460428272	-4.910000689	-2.152877835
164	H	7.238532753	0.346610558	-1.372152257	164	H	7.173531008	0.91815329	-1.455473535
165	H	6.916751473	-3.925392587	-1.24039786	165	H	6.936086626	-3.206797251	-2.590984839
166	H	10.85363754	1.679864592	-2.866235268	166	H	10.74152413	2.710705467	-2.512998624
167	H	10.44802254	0.139208981	-3.659643671	167	H	10.38083423	1.45244721	-3.718401419
168	H	11.69258963	0.180887317	-2.380620522	168	H	11.62806819	1.162648168	-2.470691965

Table S7 | Cartesian coordinates for optimized ground state and CS state geometries for **D-PBI-D** dimer in TOL.

Ground state/MCH					CS state/MCH				
No.	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	N	5.549676953	1.848736581	1.050794194	1	N	-5.069578802	-4.644341514	-0.751219859
2	N	-5.536262923	1.597739111	-1.417547629	2	N	5.30502646	-0.2858565	-2.188993791
3	O	5.052659269	1.805880673	3.268667144	3	O	-4.287921016	-5.927446722	0.964820892
4	O	5.997684682	1.977328697	-1.174500717	4	O	-5.81998575	-3.387645824	-2.498455551
5	O	-6.008039004	1.992875357	0.771161179	5	O	6.13854908	-1.952287985	-0.847828591
6	O	-5.034296321	1.206436423	-3.599482492	6	O	4.444051176	1.320516574	-3.572768905
7	C	3.733070456	1.709763957	-0.587268024	7	C	-3.567728668	-3.060266833	-1.860078893
8	C	3.327921836	1.589322926	-1.892626348	8	C	-3.367252617	-2.055086673	-2.771159426
9	C	1.967417102	1.50549962	-2.200852452	9	C	-2.105336081	-1.4657907	-2.902715283
10	C	0.995572002	1.570710898	-1.220713056	10	C	-1.024404488	-1.88284223	-2.149927642
11	C	-0.440024982	1.510753816	-1.541705035	11	C	0.309544992	-1.27916881	-2.298835696
12	C	-0.898210307	1.342739463	-2.836653164	12	C	0.544738798	-0.220086398	-3.157430227
13	C	-2.263211603	1.299827392	-3.132341337	13	C	1.821254741	0.318157297	-3.326036258
14	C	-3.194642107	1.431008888	-2.13142697	14	C	2.893444053	-0.210836086	-2.648056138
15	C	-2.770660906	1.600104004	-0.798235146	15	C	2.698990606	-1.287196397	-1.7582349
16	C	-3.727871498	1.742038088	0.227801897	16	C	3.80327597	-1.858310937	-1.088697248
17	C	-3.322112585	1.884179466	1.53091381	17	C	3.614786333	-2.895369855	-0.203346655
18	C	-1.960792599	1.888829171	1.848230756	18	C	2.330791082	-3.3901355	0.032124199
19	C	-0.987405426	1.769653547	0.874652629	19	C	1.222337221	-2.88586562	-0.627427717
20	C	-1.388416398	1.628631967	-0.487000187	20	C	1.399381519	-1.815902105	-1.554227037
21	C	1.396486856	1.698211987	0.141710545	21	C	-1.206590989	-2.936898605	-1.208559614
22	C	0.449048066	1.78291825	1.200671933	22	C	-0.130214599	-3.435941162	-0.419947206
23	C	0.910490533	1.872948153	2.502379389	23	C	-0.386809933	-4.433064952	0.505073666
24	C	2.277361572	1.881925398	2.798607873	24	C	-1.667155802	-4.968450319	0.673444431
25	C	3.207374442	1.819606078	1.789660553	25	C	-2.710992401	-4.519251729	-0.096589331
26	C	2.778567017	1.743682281	0.44930196	26	C	-2.496072336	-3.506201982	-1.055040355
27	C	4.65377128	1.823542327	2.128099058	27	C	-4.059383723	-5.105941939	0.114908822
28	C	5.174936609	1.856698518	-0.293597326	28	C	-4.913613021	-3.682466707	-1.762314231
29	C	-5.172800556	1.789389504	-0.082228376	29	C	5.17134154	-1.386097275	-1.353110778
30	C	-4.637661933	1.394837012	-2.473128858	30	C	4.233757944	0.375431496	-2.866500445
31	H	4.073323768	1.560689277	-2.677799532	31	H	-4.197649171	-1.726634671	-3.383640792
32	H	1.694670384	1.397312977	-3.241074857	32	H	-1.995091601	-0.670348034	-3.627519449
33	H	-0.201184656	1.238353209	-3.656487186	33	H	-0.264765468	0.210088863	-3.731246621
34	H	-2.601619632	1.165576918	-4.152405604	34	H	1.9848616	1.14614039	-4.004962913
35	H	-4.068638155	1.995794381	2.30768096	35	H	4.469579423	-3.333767087	0.296618323
36	H	-1.68964817	1.996472078	2.889165965	36	H	2.23139828	-4.20729667	0.731576095
37	H	0.215824652	1.935120497	3.328711631	37	H	0.406680979	-4.824762626	1.125460132

38	H	2.617440811	1.937078614	3.825518338	38	H	-1.853037694	-5.742920348	1.407290583
39	N	5.520002508	-1.741144778	-1.101691757	39	N	-5.383116468	4.570820578	0.785932632
40	N	-5.584642996	-1.64208082	1.297923475	40	N	5.106131061	0.382672309	1.956388049
41	O	5.962704085	-1.803741377	1.126323202	41	O	-6.081004189	3.279493532	2.530298245
42	O	5.037368975	-1.748318186	-3.322676159	42	O	-4.65937803	5.884686713	-0.932047319
43	O	-5.098135211	-1.246748415	3.483542462	43	O	4.304415865	-1.17899515	3.425532179
44	O	-6.033474629	-2.065817319	-0.889519764	44	O	5.813592088	2.000370299	0.440260768
45	C	3.183289373	-1.760085587	-1.853269666	45	C	-3.041836494	4.480839082	0.071998323
46	C	2.260012214	-1.841752611	-2.867201748	46	C	-2.024158958	4.947881496	-0.72205164
47	C	0.891684021	-1.85028757	-2.578987452	47	C	-0.733013348	4.430183957	-0.588867708
48	C	0.421278787	-1.762900959	-1.280266039	48	C	-0.438310438	3.435546286	0.327212548
49	C	-1.017206874	-1.767334984	-0.963182564	49	C	0.926530408	2.904483464	0.49734775
50	C	-1.982952126	-1.901046305	-1.942390967	50	C	2.00675125	3.413173061	-0.202902631
51	C	-3.346320413	-1.91501387	-1.633188552	51	C	3.30130631	2.925058886	-0.014914341
52	C	-3.761888399	-1.775239722	-0.332939092	52	C	3.534431804	1.89980699	0.873847238
53	C	-2.8125152	-1.617897063	0.698098271	53	C	2.459713	1.334332505	1.590960285
54	C	-3.247591046	-1.451109075	2.027837963	54	C	2.700682804	0.279579995	2.49102317
55	C	-2.324384586	-1.309137988	3.034796428	55	C	1.660230211	-0.255763433	3.211635004
56	C	-0.956816342	-1.336476933	2.748026525	56	C	0.368558437	0.255273674	3.071269809
57	C	-0.488246656	-1.497782019	1.456055128	57	C	0.088013135	1.296904134	2.205073237
58	C	-1.428367576	-1.629182568	0.395585297	58	C	1.146844184	1.844289185	1.424831195
59	C	1.361002356	-1.66065702	-0.216183837	59	C	-1.486675066	2.919069464	1.142066481
60	C	0.949921269	-1.536120407	1.143497045	60	C	-1.262033999	1.87112865	2.08170367
61	C	1.914544317	-1.448473064	2.129036333	61	C	-2.318308153	1.432910008	2.856723607
62	C	3.277955482	-1.504087062	1.828925492	62	C	-3.593870784	1.998051599	2.75298921
63	C	3.692730586	-1.622089694	0.526285705	63	C	-3.833634039	3.001299469	1.849189221
64	C	2.745720404	-1.683061917	-0.515705036	64	C	-2.788865556	3.467229286	1.020336731
65	C	5.138748137	-1.728984288	0.242158898	65	C	-5.19274347	3.597102668	1.781779746
66	C	4.630961771	-1.745798377	-2.18421162	66	C	-4.400683269	5.053709223	-0.099604383
67	C	-4.693812157	-1.429963347	2.359521616	67	C	4.060848674	-0.268624231	2.685320244
68	C	-5.208455411	-1.842260108	-0.030840103	68	C	4.922672685	1.428136392	1.06016994
69	H	2.606720103	-1.897658362	-3.891844914	69	H	-2.238454266	5.72404469	-1.446207314
70	H	0.202666639	-1.924453045	-3.409066833	70	H	0.03890358	4.836100733	-1.227319841
71	H	-1.704117468	-2.006045691	-2.981570012	71	H	1.874825049	4.222587201	-0.906169842
72	H	-4.08635558	-2.039407533	-2.414136197	72	H	4.132919803	3.354799631	-0.558115585
73	H	-2.671003916	-1.178102991	4.052500716	73	H	1.861015465	-1.064114504	3.904209211
74	H	-0.266484134	-1.224970339	3.572614953	74	H	-0.414402965	-0.1817776	3.675792977
75	H	1.633675358	-1.341277781	3.167176257	75	H	-2.177684875	0.639378227	3.578168029
76	H	4.018523586	-1.4512217	2.617488895	76	H	-4.404857142	1.652452932	3.38188221
77	C	-6.941689196	1.680993373	-1.733525402	77	C	6.605665746	0.258015331	-2.37889975
78	C	-7.470020142	2.927709365	-2.044247958	78	C	7.299681787	-0.115317773	-3.528535807

79	C	-7.722855019	0.547229841	-1.702422495	79	C	7.174922211	1.091389812	-1.445829611
80	C	-8.827002007	3.042201089	-2.318717612	80	C	8.597837427	0.324146221	-3.753434409
81	C	-9.084170566	0.666344851	-1.963025052	81	C	8.483166557	1.506308431	-1.661374185
82	C	-9.652192309	1.904497798	-2.258441634	82	C	9.202541328	1.15741636	-2.800139636
83	O	-9.446052104	4.200203849	-2.648938553	83	O	9.364799124	-0.015311723	-4.823228812
84	O	-10.98464925	1.963055552	-2.519979901	84	O	10.4754819	1.616518679	-2.990989349
85	O	-9.865325122	-0.447079912	-1.860863334	85	O	9.105027374	2.284021646	-0.714100737
86	C	-8.671381304	5.384144434	-2.683112489	86	C	8.796792513	-0.875501654	-5.778094427
87	C	-10.3709325	-0.944277755	-3.095451696	87	C	8.99760646	3.668182734	-0.972705885
88	C	-11.76707503	2.838730053	-1.70941893	88	C	11.45953731	0.871451602	-2.28438209
89	H	-6.816019317	3.788019953	-2.066557996	89	H	6.771486963	-0.76813996	-4.208874073
90	H	-7.318210742	-0.423556873	-1.448407227	90	H	6.590312489	1.461988507	-0.513291588
91	H	-9.360214946	6.182545006	-2.95102412	91	H	9.559925622	-1.029040616	-6.539619542
92	H	-7.880530748	5.31749801	-3.437471303	92	H	7.907344084	-0.43232058	-6.242822907
93	H	-8.229348033	5.598058455	-1.704264936	93	H	8.524604455	-1.843713873	-5.33925453
94	H	-10.94332909	-1.838586703	-2.853023899	94	H	9.502107883	4.182592652	-0.154156937
95	H	-9.546394038	-1.209536968	-3.765537218	95	H	7.944545741	3.974293049	-0.999962701
96	H	-11.02050796	-0.210706585	-3.578427835	96	H	9.481417541	3.92928313	-1.920609528
97	H	-12.75743819	2.388930381	-1.635074663	97	H	12.41899721	1.337360061	-2.507663558
98	H	-11.836171121	3.826939989	-2.166139514	98	H	11.4772203	-0.168456536	-2.627700996
99	H	-11.33282532	2.929470672	-0.710503983	99	H	11.27301325	0.90031616	-1.206581844
100	C	-6.990369292	-1.743809149	1.613886263	100	C	6.396828715	-0.17767598	2.178210102
101	C	-7.775896486	-0.612505812	1.615456668	101	C	6.920805273	-1.24354261	1.465815893
102	C	-7.504407968	-3.004210767	1.893913049	102	C	7.099704293	0.418846991	3.219253667
103	C	-9.130544586	-0.735253321	1.922718312	103	C	8.189501862	-1.715007263	1.852622613
104	C	-8.853898157	-3.124942723	2.2005791	104	C	8.358356495	-0.028768773	3.57598229
105	C	-9.673414146	-1.983379076	2.218669056	105	C	8.912367424	-1.103817821	2.878469436
106	O	-9.870689474	0.404815241	1.992199233	106	O	8.779027961	-2.824988856	1.34054122
107	O	-10.99293308	-2.124787768	2.541404973	107	O	10.17675005	-1.520409876	3.185372402
108	O	-9.467889275	-4.286242499	2.518155479	108	O	9.115255353	0.491354289	4.578614533
109	C	-11.27013272	-1.825152241	3.90623375	109	C	10.21381899	-2.672443496	4.005113289
110	C	-11.04737544	0.468095391	1.182715234	110	C	8.656273281	-3.089185028	-0.053978277
111	C	-8.685197196	-5.464564185	2.527813549	111	C	8.646064797	1.659618031	5.202543368
112	H	-7.367748408	0.360707202	1.376058906	112	H	6.347603541	-1.698949577	0.593623481
113	H	-6.84759194	-3.862495663	1.874947797	113	H	6.603581485	1.239721972	3.714998355
114	H	-12.33375339	-2.008073841	4.055673801	114	H	11.26649825	-2.897509944	4.182319277
115	H	-11.03994207	-0.778060808	4.12806868	115	H	9.739535249	-3.52368913	3.506220153
116	H	-10.69168603	-2.478073177	4.567269164	116	H	9.719804168	-2.484306033	4.966242743
117	H	-11.34718974	1.515591116	1.185258294	117	H	8.946769594	-4.132828729	-0.190836974
118	H	-11.84800701	-0.146916978	1.596799687	118	H	9.358302818	-2.460536015	-0.60150337
119	H	-10.82933177	0.147762746	0.160747722	119	H	7.644205446	-2.911150829	-0.444339765

120	H	-9.364576172	-6.270174871	2.798577066	120	H	9.41317084	1.949393846	5.919636353
121	H	-7.880436612	-5.401381158	3.268326389	121	H	7.703474174	1.48636164	5.737566711
122	H	-8.258743484	-5.667249444	1.539560658	122	H	8.502169198	2.471328067	4.478895859
123	C	6.962319339	1.96332946	1.338135403	123	C	-6.358554051	-5.23709355	-0.607992298
124	C	7.508213972	3.239052541	1.445350096	124	C	-6.630971865	-6.414395859	-1.291531836
125	C	7.72506859	0.824444488	1.449195114	125	C	-7.315130393	-4.627434304	0.17050807
126	C	8.871431291	3.357749918	1.677674106	126	C	-7.88552599	-6.997769069	-1.178295723
127	C	9.098621625	0.945675552	1.670854201	127	C	-8.584342815	-5.193858686	0.275464797
128	C	9.674083325	2.206792022	1.782216177	128	C	-8.873043905	-6.383886995	-0.390268543
129	O	9.526522961	4.530376738	1.835930932	129	O	-8.250081038	-8.162483999	-1.761216477
130	O	11.01608613	2.35432366	2.004260221	130	O	-10.09930284	-6.977694891	-0.281376033
131	O	9.802694749	-0.203072683	1.819960787	131	O	-9.481886996	-4.570158035	1.082571198
132	C	11.34176765	2.42558098	3.390856157	132	C	-10.22908463	-7.770794951	0.88957937
133	C	11.03400098	-0.34252185	1.108173202	133	C	-10.79809247	-4.349435946	0.583650469
134	C	8.771913593	5.724040503	1.750676717	134	C	-7.298205226	-8.813031151	-2.571819892
135	H	6.866837227	4.103115609	1.34554213	135	H	-5.840669556	-6.847084396	-1.886745223
136	H	7.294196343	-0.163750417	1.360146243	136	H	-7.092591099	-3.706090497	0.690637303
137	H	12.42514708	2.33271461	3.46876284	137	H	-11.22855527	-8.204811155	0.864573754
138	H	10.86482515	1.61171737	3.944382303	138	H	-10.11569266	-7.159562916	1.792319691
139	H	11.02541755	3.389184685	3.803966669	139	H	-9.485893439	-8.574621218	0.897534086
140	H	11.15218729	-1.408481694	0.914222696	140	H	-11.13694228	-3.413625301	1.028743089
141	H	11.87449632	0.029377544	1.696602046	141	H	-11.47288	-5.159285322	0.867140326
142	H	10.98967304	0.190771336	0.157649803	142	H	-10.79290074	-4.25339551	-0.504670618
143	H	9.479947212	6.534787805	1.909785802	143	H	-7.786596585	-9.709588461	-2.94910306
144	H	7.996196865	5.762427747	2.523115252	144	H	-6.409830297	-9.100599592	-1.997123588
145	H	8.310717767	5.831912316	0.76319191	145	H	-6.994785817	-8.185217142	-3.41743242
146	C	11.54967433	-2.767249237	-3.025918773	146	C	-10.67315839	8.046000766	-0.010823307
147	C	8.844162357	-5.558775118	-1.269677725	147	C	-7.771637511	8.397334568	3.073005868
148	C	6.935400549	-1.838893432	-1.37394241	148	C	-6.682181824	5.147333635	0.677638894
149	C	7.674455482	-0.696975329	-1.567068477	149	C	-7.621314466	4.585628618	-0.153560538
150	C	7.516111468	-3.101594569	-1.387246072	150	C	-6.986640563	6.264088576	1.443168911
151	C	9.049317477	-0.801232151	-1.783831461	151	C	-8.898368337	5.140116352	-0.244455214
152	C	8.88674098	-3.205373691	-1.573565728	152	C	-8.258575005	6.812360185	1.380139634
153	C	9.66983961	-2.05071013	-1.775592347	153	C	-9.229182297	6.258486159	0.523679961
154	O	9.713664534	0.375860163	-1.907819891	154	O	-9.777902237	4.483650848	-1.044202937
155	O	11.03016491	-2.137944776	-1.856627702	155	O	-10.50762573	6.737487603	0.519518727
156	O	9.569474781	-4.373979347	-1.539398313	156	O	-8.673326467	7.864494571	2.128263529
157	C	10.74108994	0.499392828	-2.883069093	157	C	-10.62015795	5.233400373	-1.90539204
158	H	12.63182457	-2.649486573	-2.979072074	158	H	-11.74661113	8.233908769	-0.029678788
159	H	11.1682931	-2.277361977	-3.928093065	159	H	-10.27613819	8.104174528	-1.031257037
160	H	11.29468918	-3.827514458	-3.048676386	160	H	-10.18149824	8.79160083	0.616273183

161	H	9.576901029	-6.3631174	-1.26616665	161	H	-8.309878051	9.19132801	3.587344938
162	H	8.095720465	-5.752954488	-2.045108558	162	H	-6.882408601	8.81782076	2.589593795
163	H	8.354495669	-5.508971928	-0.291727105	163	H	-7.46569462	7.638139519	3.801104746
164	H	7.232068341	0.289074437	-1.530279453	164	H	-7.385354497	3.700523618	-0.727879629
165	H	6.898908699	-3.97158856	-1.214652115	165	H	-6.21824069	6.657296671	2.091793927
166	H	10.85384739	1.568191938	-3.061450284	166	H	-10.94220228	4.541617835	-2.683616543
167	H	10.44814257	0.008414882	-3.816622297	167	H	-10.06792693	6.058697485	-2.368961454
168	H	11.68350212	0.082475691	-2.526349422	168	H	-11.48932502	5.62612178	-1.37713963

Table S8 | Cartesian coordinates for optimized ground state and CS state geometries for **D-PBI-D** dimer in DEE.

Ground state/MCH					CS state/MCH				
No.	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	N	5.550199253	1.838213144	1.136714437	1	N	-5.352453346	-1.807539311	-0.405202838
2	N	-5.546185118	1.574672875	-1.285884884	2	N	5.782103287	-0.740435037	-2.325878057
3	O	5.060841919	1.790348539	3.354496461	3	O	-4.895264952	-2.925095252	1.535040009
4	O	5.99047642	1.958851452	-1.095329175	4	O	-5.756811544	-0.631588709	-2.317998706
5	O	-6.002590869	1.98538185	0.905572115	5	O	6.227151488	-2.153054635	-0.588170218
6	O	-5.053914442	1.201751942	-3.472331305	6	O	5.331110454	0.545466824	-4.158884494
7	C	3.729391151	1.705104327	-0.497200055	7	C	-3.494075007	-1.036225641	-1.804907221
8	C	3.317809139	1.590385984	-1.801638035	8	C	-3.053377723	-0.42107114	-2.947845765
9	C	1.956187121	1.510836304	-2.105571169	9	C	-1.683758739	-0.303697958	-3.196892243
10	C	0.988655111	1.573244918	-1.121006668	10	C	-0.740953223	-0.78907543	-2.312689912
11	C	-0.448173611	1.516347396	-1.437767782	11	C	0.69877553	-0.603813519	-2.534375472
12	C	-0.910928065	1.366729373	-2.733122858	12	C	1.180842365	0.144200545	-3.593216032
13	C	-2.277621516	1.318192832	-3.022504591	13	C	2.54924379	0.2961961	-3.81789881
14	C	-3.205337451	1.431926501	-2.01575977	14	C	3.460271328	-0.30636438	-2.984114718
15	C	-2.775703394	1.591108142	-0.682881728	15	C	3.013829603	-1.069915923	-1.885504713
16	C	-3.728155035	1.726977919	0.347706587	16	C	3.9502963	-1.707780358	-1.041831462
17	C	-3.316717639	1.856488318	1.651150065	17	C	3.510584063	-2.45146818	0.029692803
18	C	-1.954777376	1.855809021	1.963354482	18	C	2.143580323	-2.563800811	0.29680617
19	C	-0.986166989	1.74580492	0.983469058	19	C	1.19047874	-1.959390186	-0.504505779
20	C	-1.392369462	1.617632032	-0.37735677	20	C	1.624940881	-1.209678991	-1.637582736
21	C	1.395109368	1.691577383	0.240579435	21	C	-1.176422201	-1.476895525	-1.144705558
22	C	0.451363847	1.763028347	1.303907398	22	C	-0.255954833	-2.062997152	-0.230430683
23	C	0.915931099	1.844165104	2.604843529	23	C	-0.753465944	-2.713676404	0.885295238
24	C	2.283582809	1.857570518	2.895621248	24	C	-2.126142738	-2.802879356	1.133736022
25	C	3.210260508	1.806354807	1.882581057	25	C	-3.027808043	-2.245452246	0.260700969
26	C	2.778296904	1.736834924	0.543319556	26	C	-2.567139534	-1.586414482	-0.895302217
27	C	4.656222396	1.816796923	2.215085637	27	C	-4.480685643	-2.37167657	0.549750525
28	C	5.171132406	1.844005946	-0.208434181	28	C	-4.954029278	-1.117971352	-1.561060495
29	C	-5.173594296	1.774293076	0.045544568	29	C	5.398025104	-1.572057992	-1.288334368
30	C	-4.649540374	1.39187004	-2.348008316	30	C	4.902260828	-0.110004496	-3.250399445
31	H	4.057389308	1.56203494	-2.592188478	31	H	-3.780170389	-0.01675808	-3.641786817
32	H	1.680217664	1.404298615	-3.145088168	32	H	-1.377364988	0.190199627	-4.109263293
33	H	-0.218662329	1.281011457	-3.559141861	33	H	0.498870723	0.626488416	-4.280289745
34	H	-2.616607476	1.19451625	-4.043619833	34	H	2.910889124	0.884212536	-4.652874196
35	H	-4.058439429	1.962614811	2.432915373	35	H	4.231863306	-2.955214183	0.66138674
36	H	-1.679136115	1.953764694	3.003951491	36	H	1.849257705	-3.154489095	1.152276295
37	H	0.224753799	1.893791253	3.434745015	37	H	-0.08253205	-3.165743142	1.601687336

38	H	2.624617996	1.905630654	3.922398293	38	H	-2.500066725	-3.312209907	2.013318827
39	N	5.529488264	-1.769632999	-0.920008732	39	N	-5.770121133	2.073105222	0.578659208
40	N	-5.618764263	-1.669546067	1.23618602	40	N	5.394185273	0.390175356	1.927603695
41	O	5.925456011	-1.800471444	1.321225278	41	O	-6.056535612	1.207836403	2.699528912
42	O	5.096817234	-1.795059673	-3.149643546	42	O	-5.329508169	3.059922136	-1.441694457
43	O	-5.1868385	-1.284859528	3.432743699	43	O	4.97704867	-0.772808653	3.854393595
44	O	-6.021526253	-2.11992391	-0.953614792	44	O	5.781720497	1.62998398	0.037426481
45	C	3.21061529	-1.80081546	-1.721582354	45	C	-3.448118822	2.335367527	-0.228999502
46	C	2.309549557	-1.881242142	-2.755757384	46	C	-2.567457179	2.798343703	-1.175428296
47	C	0.935399516	-1.885315674	-2.498318178	47	C	-1.192472863	2.594995238	-1.020814415
48	C	0.437969905	-1.796053678	-1.209967686	48	C	-0.67301266	1.924815412	0.072019773
49	C	-1.00716749	-1.794413287	-0.923959973	49	C	0.775004882	1.72150826	0.261003027
50	C	-1.950580043	-1.922407336	-1.925844193	50	C	1.712815729	2.239454821	-0.615997124
51	C	-3.319475612	-1.939511886	-1.646015552	51	C	3.082400563	2.046630596	-0.426019323
52	C	-3.762874509	-1.807596621	-0.353700398	52	C	3.535278487	1.32179012	0.650622495
53	C	-2.837452781	-1.651863137	0.69853001	53	C	2.620104478	0.772076692	1.571243137
54	C	-3.300722518	-1.492162366	2.02041035	54	C	3.088926496	0.026340841	2.673489235
55	C	-2.39898837	-1.355891764	3.047305778	55	C	2.193866438	-0.524478993	3.557480278
56	C	-1.025299746	-1.383822673	2.790069498	56	C	0.82204279	-0.326439821	3.386141516
57	C	-0.530573673	-1.53592541	1.507181134	57	C	0.321452652	0.431400518	2.34293372
58	C	-1.44738496	-1.659554015	0.425476296	58	C	1.228565899	0.975180649	1.388687874
59	C	1.354282142	-1.697923221	-0.125104091	59	C	-1.572388161	1.421363666	1.054865646
60	C	0.913405013	-1.572735513	1.224926581	60	C	-1.116990124	0.695141097	2.191613454
61	C	1.854867576	-1.483638184	2.232371124	61	C	-2.041882352	0.262881121	3.12391738
62	C	3.224282274	-1.535018657	1.961941776	62	C	-3.407611842	0.517361951	2.978931426
63	C	3.66892477	-1.652512383	0.668708502	63	C	-3.868139267	1.198962257	1.879122445
64	C	2.745249075	-1.720055962	-0.394029128	64	C	-2.961842626	1.651667596	0.900490119
65	C	5.120063135	-1.746278054	0.417080983	65	C	-5.318001353	1.486362669	1.780472371
66	C	4.663547684	-1.79199754	-2.01979715	66	C	-4.904914985	2.533366678	-0.446713407
67	C	-4.752986657	-1.475207911	2.319681277	67	C	4.536426831	-0.175586006	2.91167022
68	C	-5.212886746	-1.88184479	-0.081803136	68	C	4.984136023	1.134970811	0.826653387
69	H	2.676355132	-1.938717437	-3.77310655	69	H	-2.957636897	3.311292832	-2.045427736
70	H	0.265649557	-1.95545806	-3.344078849	70	H	-0.53703245	2.975541211	-1.792274246
71	H	-1.648084614	-2.020366264	-2.958900021	71	H	1.402756421	2.821342368	-1.472336126
72	H	-4.0409719	-2.061997715	-2.444192809	72	H	3.800211144	2.468663105	-1.119416178
73	H	-2.76431805	-1.231993266	4.059246911	73	H	2.569647648	-1.100995189	4.39423436
74	H	-0.353754365	-1.281533831	3.631282966	74	H	0.153416615	-0.775160581	4.107951207
75	H	1.550722111	-1.376305924	3.263953078	75	H	-1.723837006	-0.284527552	4.000545762
76	H	3.944645887	-1.478168906	2.768549311	76	H	-4.114000268	0.184861536	3.729290142
77	C	-6.952930261	1.655615984	-1.59920337	77	C	7.146828209	-0.341629503	-2.381878283
78	C	-7.498225624	2.906200698	-1.849954156	78	C	7.999790984	-0.881904276	-3.33491226

79	C	-7.720786677	0.510100028	-1.638807475	79	C	7.576688411	0.592674412	-1.457766329
80	C	-8.85236445	3.017108487	-2.145289124	80	C	9.341817573	-0.519595728	-3.338308465
81	C	-9.08299535	0.626615405	-1.885855165	81	C	8.921980079	0.933153393	-1.453668155
82	C	-9.670338639	1.872783981	-2.129959833	82	C	9.813489139	0.386247349	-2.375255316
83	O	-9.457133645	4.184430139	-2.471731478	83	O	10.27430025	-1.01849236	-4.190135599
84	O	-10.99724231	1.894153804	-2.412388474	84	O	11.14114026	0.704239788	-2.327552252
85	O	-9.85386779	-0.498568268	-1.848205271	85	O	9.39055858	1.770386663	-0.476596506
86	C	-8.698658591	5.37755115	-2.380583736	86	C	9.83793055	-1.958744049	-5.139740202
87	C	-10.2666625	-0.982045514	-3.121487866	87	C	9.760751474	3.05985399	-0.928536899
88	C	-11.810212	2.899337472	-1.810035429	88	C	11.84598336	-0.049629621	-1.342570471
89	H	-6.85847841	3.777624716	-1.832120805	89	H	7.57899271	-1.575346088	-4.04924596
90	H	-7.291213505	-0.468297792	-1.463793513	90	H	6.80879268	1.037131242	-0.724207357
91	H	-9.383258673	6.18358746	-2.635842158	91	H	10.71797179	-2.238140859	-5.717005577
92	H	-7.863601964	5.373986379	-3.088441598	92	H	9.085459741	-1.532106875	-5.814189529
93	H	-8.318652067	5.527788509	-1.364972987	93	H	9.421518776	-2.853523084	-4.660045171
94	H	-10.8509632	-1.88228757	-2.935986812	94	H	10.11333293	3.603342766	-0.05182331
95	H	-9.395743761	-1.235178956	-3.73572954	95	H	8.895326365	3.581363675	-1.355777312
96	H	-10.88439568	-0.246621289	-3.642995144	96	H	10.56270419	3.007550234	-1.671006084
97	H	-12.8257167	2.505179979	-1.823134852	97	H	12.8581196	0.353915062	-1.31072317
98	H	-11.75916895	3.834802862	-2.363427293	98	H	11.88628647	-1.106257646	-1.630591808
99	H	-11.50467565	3.079521271	-0.774596587	99	H	11.37926229	0.044332649	-0.357382171
100	C	-7.034712823	-1.75815625	1.505159347	100	C	6.79202574	0.183077957	2.097242338
101	C	-7.794406387	-0.612428881	1.519151975	101	C	7.403079797	-0.812380992	1.375257736
102	C	-7.58672165	-3.019362135	1.696844604	102	C	7.497539539	0.976172104	2.990008895
103	C	-9.16922776	-0.715527931	1.734590686	103	C	8.774032911	-1.018000335	1.523034882
104	C	-8.954346173	-3.121290727	1.913386591	104	C	8.864629626	0.782742997	3.135765097
105	C	-9.754036027	-1.964837194	1.931581166	105	C	9.514898431	-0.201618311	2.378878196
106	O	-9.86344725	0.448661053	1.796867171	106	O	9.44908824	-2.021826643	0.91393321
107	O	-11.09258949	-2.104766965	2.170683364	107	O	10.87264491	-0.322866317	2.467680494
108	O	-9.610526165	-4.281868882	2.138607968	108	O	9.65698435	1.496072515	3.977469491
109	C	-11.448696	-1.82945136	3.522747622	109	C	11.29965348	-1.390525691	3.293977767
110	C	-11.07040203	0.585555385	1.046521598	110	C	9.033355217	-2.441369825	-0.390347173
111	C	-8.850708006	-5.477555509	2.160828685	111	C	9.049495808	2.525312854	4.716020658
112	H	-7.359791415	0.361520885	1.336140154	112	H	6.795486359	-1.401507025	0.649099119
113	H	-6.948060222	-3.890677542	1.670488754	113	H	6.93675144	1.705691314	3.556041853
114	H	-12.51667389	-2.025213183	3.612389104	114	H	12.38999865	-1.36588059	3.299018307
115	H	-11.24428452	-0.782985085	3.775724065	115	H	10.95657646	-2.350992337	2.89762477
116	H	-10.89807597	-2.482860848	4.206374168	116	H	10.9319425	-1.258863067	4.318541144
117	H	-11.19412483	1.657840544	0.898101124	117	H	9.385603325	-3.469026296	-0.495289253
118	H	-11.93264078	0.201255111	1.595070368	118	H	9.533446898	-1.820710726	-1.136720912
119	H	-10.98522383	0.092105546	0.076334394	119	H	7.936911603	-2.371568311	-0.548654617

120	H	-9.560212864	-6.275746385	2.368524061	120	H	9.842850827	2.985708221	5.303218303
121	H	-8.091300532	-5.450922305	2.949326385	121	H	8.278376901	2.138283351	5.393997788
122	H	-8.37004423	-5.660355825	1.194164921	122	H	8.600948017	3.281574425	4.060260387
123	C	6.959994573	1.952505312	1.43385579	123	C	-6.75180105	-2.031808746	-0.220384799
124	C	7.51872824	3.221544964	1.500185746	124	C	-7.380568637	-2.926599121	-1.07899041
125	C	7.720220676	0.816691798	1.608031929	125	C	-7.444563511	-1.408751114	0.792409363
126	C	8.880300828	3.349541646	1.749932721	126	C	-8.726236058	-3.213570145	-0.908392445
127	C	9.087997014	0.943779961	1.83508725	127	C	-8.793461188	-1.706978531	0.981077413
128	C	9.682814681	2.20532292	1.908960588	128	C	-9.438954152	-2.608307407	0.138618259
129	O	9.51287369	4.539535222	1.884059447	129	O	-9.431961871	-4.08293415	-1.668536644
130	O	11.01002536	2.266724245	2.191788191	130	O	-10.75542271	-2.924511136	0.321823839
131	O	9.796210808	-0.201282002	2.01888225	131	O	-9.422860698	-1.140189997	2.043034322
132	C	11.85112531	2.956573274	1.270625331	132	C	-10.94350058	-4.018910646	1.206129453
133	C	10.97730448	-0.387271848	1.233865048	133	C	-10.67954906	-0.515955685	1.797001518
134	C	8.753553871	5.720498421	1.700881542	134	C	-8.768763418	-4.685704351	-2.755799735
135	H	6.888516224	4.088691753	1.359943609	135	H	-6.792602576	-3.370529311	-1.869084889
136	H	7.29793889	-0.176060751	1.541069036	136	H	-6.961136669	-0.704112161	1.458327236
137	H	12.85540062	2.561503178	1.424729222	137	H	-12.01835263	-4.188758455	1.26984534
138	H	11.83624828	4.030453992	1.451762397	138	H	-10.54865004	-3.7872884	2.201765287
139	H	11.54015452	2.75289734	0.239952125	139	H	-10.45782452	-4.919855879	0.817389962
140	H	11.07187425	-1.459820343	1.064590368	140	H	-10.81535886	0.206965517	2.600438567
141	H	11.85530592	-0.01245103	1.762196834	141	H	-11.49630071	-1.239725292	1.802723885
142	H	10.87592125	0.113326211	0.268966125	142	H	-10.67199757	0.006565663	0.83764803
143	H	9.450850933	6.544806918	1.835041096	143	H	-9.507552528	-5.319006985	-3.243544265
144	H	7.953412445	5.798217687	2.44399855	144	H	-7.927282658	-5.304695151	-2.422255115
145	H	8.325160238	5.765020051	0.694290616	145	H	-8.408513514	-3.935655621	-3.468899183
146	C	11.56776932	-2.854197801	-2.769180011	146	C	-11.79637971	4.075739944	-0.200022122
147	C	8.870127867	-5.582018049	-0.986795645	147	C	-9.630547382	3.737299191	3.408501294
148	C	6.94873218	-1.866181102	-1.172311402	148	C	-7.171265446	2.267745535	0.372684843
149	C	7.686391466	-0.726079119	-1.387560657	149	C	-7.736367163	1.926172611	-0.836984632
150	C	7.532142898	-3.127562566	-1.153933895	150	C	-7.957226954	2.807758311	1.388848009
151	C	9.062257009	-0.832247629	-1.597878725	151	C	-9.092495924	2.148351031	-1.065441798
152	C	8.904318977	-3.231842529	-1.33067793	152	C	-9.312480406	2.994064036	1.181759434
153	C	9.684924394	-2.080741708	-1.557424285	153	C	-9.898011044	2.680230082	-0.055892908
154	O	9.720265734	0.345422966	-1.750971342	154	O	-9.560019729	1.755894831	-2.279256339
155	O	11.04475271	-2.170783622	-1.631096118	155	O	-11.25027713	2.765674188	-0.230753412
156	O	9.592646214	-4.395082762	-1.266575547	156	O	-10.17208407	3.422205463	2.144841503
157	C	10.76724311	0.453175128	-2.710628494	157	C	-10.48575972	2.581448317	-2.963177723
158	H	12.64938075	-2.731722052	-2.726634384	158	H	-12.84709996	3.974284714	-0.471903321
159	H	11.18506681	-2.410194324	-3.693911076	159	H	-11.29334342	4.723263717	-0.928229155
160	H	11.31444834	-3.914830594	-2.739537888	160	H	-11.71506521	4.515783071	0.795636015

161	H	9.607939731	-6.3809811	-0.960620039	161	H	-10.47098478	4.046023487	4.027944984
162	H	8.133091878	-5.791047528	-1.768536979	162	H	-8.907032082	4.557587867	3.338047693
163	H	8.368674791	-5.519172479	-0.01588196	163	H	-9.147269359	2.868385886	3.866027138
164	H	7.243918422	0.260850208	-1.374520197	164	H	-7.118964105	1.505866454	-1.614685511
165	H	6.9161096	-3.995138134	-0.965980963	165	H	-7.493819917	2.942541496	2.350174495
166	H	10.84938145	1.514879623	-2.941421736	166	H	-10.39984571	2.317517996	-4.017788978
167	H	10.51355271	-0.092955584	-3.623944801	167	H	-10.23016425	3.640328708	-2.841223156
168	H	11.71237528	0.084970268	-2.310665762	168	H	-11.5074768	2.411749317	-2.621180501

Table S9 | Cartesian coordinates for optimized ground state and CS state geometries for **D-PBI-D** dimer in THF.

Ground state/MCH					CS state/MCH				
No.	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	N	5.559891295	1.843130289	1.081599461	1	N	5.525783273	1.6178771	1.409650666
2	N	-5.551355467	1.589475329	-1.264388648	2	N	-5.541672342	1.821777626	-1.19565216
3	O	5.087870991	1.84751888	3.303761085	3	O	4.997027903	1.169691707	3.57814779
4	O	5.993342731	1.931338738	-1.145364797	4	O	5.995583161	2.120489089	-0.758950179
5	O	-5.996568439	1.983303222	0.932775704	5	O	-6.034974403	1.844750887	1.024850528
6	O	-5.074594257	1.240663491	-3.457318756	6	O	-4.998972978	1.788419403	-3.405547776
7	C	3.728616421	1.687815122	-0.535423979	7	C	3.723308606	1.79511139	-0.243300109
8	C	3.307561971	1.554830571	-1.835666347	8	C	3.332585034	1.950312679	-1.548459089
9	C	1.944001187	1.478071229	-2.130020068	9	C	1.975207751	1.937773164	-1.881044686
10	C	0.983265118	1.563850222	-1.140113148	10	C	0.991578589	1.797049252	-0.92120036
11	C	-0.455775936	1.517113414	-1.447874367	11	C	-0.43987445	1.797147456	-1.264362704
12	C	-0.926141315	1.363330446	-2.739898335	12	C	-0.884008723	1.888415677	-2.571957516
13	C	-2.294672059	1.321974806	-3.021027884	13	C	-2.24509636	1.885192115	-2.887496086
14	C	-3.21603523	1.44125325	-2.008849578	14	C	-3.187049301	1.806317093	-1.89170324
15	C	-2.778358391	1.604737024	-0.67895491	15	C	-2.778739654	1.726261408	-0.54604565
16	C	-3.724100622	1.74192039	0.357827202	16	C	-3.750801088	1.664569147	0.473564862
17	C	-3.303145311	1.876820562	1.657982858	17	C	-3.361721936	1.538871348	1.783009292
18	C	-1.939156806	1.882546644	1.960800663	18	C	-2.003441107	1.475362278	2.110762195
19	C	-0.977414554	1.769027379	0.974439822	19	C	-1.015648271	1.562384635	1.148347859
20	C	-1.392990309	1.631286468	-0.382513677	20	C	-1.400227215	1.695668388	-0.218883362
21	C	1.399091491	1.69657418	0.21704903	21	C	1.377176228	1.647247005	0.443318473
22	C	0.46252577	1.78734163	1.28539328	22	C	0.417742087	1.513772565	1.486466986
23	C	0.935469458	1.886525909	2.582323492	23	C	0.868092358	1.340104995	2.783387652
24	C	2.304983842	1.898954263	2.864361614	24	C	2.231833996	1.2965695	3.091236658
25	C	3.225119203	1.825868395	1.846193205	25	C	3.172460128	1.439097048	2.101250888
26	C	2.784370031	1.73825819	0.510446628	26	C	2.756335842	1.625992866	0.768310269
27	C	4.672502974	1.827671128	2.166736038	27	C	4.618132086	1.386006977	2.453577665
28	C	5.172419909	1.830099231	-0.258039392	28	C	5.166832082	1.862204344	0.082994616
29	C	-5.171020113	1.783853386	0.065333318	29	C	-5.194829106	1.780695326	0.158141015
30	C	-4.661333483	1.399475966	-2.330514459	30	C	-4.626580511	1.79675326	-2.257435733
31	H	4.040534301	1.510828659	-2.631428733	31	H	4.090055242	2.084101566	-2.311059127
32	H	1.661516282	1.358997654	-3.166376114	32	H	1.713947666	2.052221884	-2.923850549
33	H	-0.239545251	1.267595463	-3.569438189	33	H	-0.176694415	1.962313267	-3.38657778
34	H	-2.638235738	1.193866323	-4.039968387	34	H	-2.578088413	1.943801452	-3.916725905
35	H	-4.038135338	1.982398899	2.446019846	35	H	-4.120954363	1.48474712	2.554030308
36	H	-1.656921907	1.984431706	2.999160194	36	H	-1.74437263	1.359650362	3.153984139
37	H	0.250361013	1.952221276	3.415965565	37	H	0.16297147	1.228118641	3.595869927

38	H	2.65038406	1.960286217	3.888829409	38	H	2.566257813	1.151300443	4.111411403
39	N	5.536250872	-1.772123537	-0.867209405	39	N	5.509412038	-1.534163628	-1.421025885
40	N	-5.62785486	-1.678268534	1.196557675	40	N	-5.558448581	-1.790358255	1.162616804
41	O	5.919450602	-1.773962229	1.371193421	41	O	5.982477417	-2.010106752	0.752349928
42	O	5.125007059	-1.824724023	-3.099982702	42	O	4.984266	-1.11228747	-3.595621563
43	O	-5.212629434	-1.32807722	3.401458068	43	O	-5.019043831	-1.798894986	3.373556727
44	O	-6.016590135	-2.107968602	-1.001109479	44	O	-6.047790531	-1.794534516	-1.05846645
45	C	3.223939279	-1.798567439	-1.690946747	45	C	3.158138502	-1.390080588	-2.12052081
46	C	2.331141851	-1.878373734	-2.732918871	46	C	2.218109085	-1.256623599	-3.11251898
47	C	0.954886429	-1.879582051	-2.486923114	47	C	0.854590781	-1.309000198	-2.806807309
48	C	0.447510163	-1.794253744	-1.202003885	48	C	0.403575282	-1.484303136	-1.51019215
49	C	-1.000020924	-1.794438376	-0.927855594	49	C	-1.029793065	-1.537295255	-1.173934308
50	C	-1.935135691	-1.914112743	-1.938768285	50	C	-2.016053155	-1.451002031	-2.137757987
51	C	-3.306243914	-1.931500596	-1.669688439	51	C	-3.374615628	-1.512597661	-1.811280687
52	C	-3.76102817	-1.807914971	-0.380056756	52	C	-3.764489809	-1.638835587	-0.502349792
53	C	-2.843608758	-1.661728889	0.680620346	53	C	-2.794054913	-1.703901701	0.518365892
54	C	-3.316298451	-1.509741303	2.000067963	54	C	-3.204403373	-1.78829347	1.86311433
55	C	-2.422705227	-1.387050107	3.036010578	55	C	-2.263941854	-1.870228458	2.859863906
56	C	-1.047296096	-1.413025267	2.78946116	56	C	-0.902368589	-1.869218	2.546022039
57	C	-0.543490589	-1.551804435	1.508636659	57	C	-0.456736183	-1.772922159	1.239382164
58	C	-1.451438526	-1.669686289	0.418760166	58	C	-1.415579348	-1.67206693	0.192729131
59	C	1.354742861	-1.698623991	-0.109313376	59	C	1.361839954	-1.61210888	-0.465496054
60	C	0.902605861	-1.578970546	1.237326056	60	C	0.974931852	-1.764673766	0.898527963
61	C	1.835207128	-1.48482618	2.252720225	61	C	1.957207089	-1.896808155	1.860982813
62	C	3.206551476	-1.528017797	1.992710225	62	C	3.315020184	-1.894215271	1.531983393
63	C	3.66267587	-1.645039515	0.702998549	63	C	3.706137128	-1.736525502	0.227125761
64	C	2.747777079	-1.717003284	-0.367023377	64	C	2.741239918	-1.578944488	-0.787889143
65	C	5.116055118	-1.734181921	0.463693623	65	C	5.149619389	-1.776466494	-0.09269045
66	C	4.678451299	-1.789570666	-1.974724766	66	C	4.602691715	-1.323894111	-2.470813983
67	C	-4.769407528	-1.483388099	2.285603886	67	C	-4.64508893	-1.786092164	2.226723359
68	C	-5.213397091	-1.880321679	-0.120691482	68	C	-5.209168896	-1.745056371	-0.187751371
69	H	2.704073983	-1.933900685	-3.747996265	69	H	2.552995438	-1.110205027	-4.132363449
70	H	0.292287084	-1.945938051	-3.33852848	70	H	0.149993989	-1.201825419	-3.620287747
71	H	-1.62488331	-2.004844383	-2.97018212	71	H	-1.755767868	-1.334206682	-3.180531264
72	H	-4.019973665	-2.046010638	-2.475785882	72	H	-4.133730517	-1.454173065	-2.582045829
73	H	-2.793945428	-1.269132703	4.04641948	73	H	-2.598476286	-1.93422067	3.888252173
74	H	-0.382824286	-1.316909287	3.636717377	74	H	-0.196134975	-1.944151787	3.361457477
75	H	1.522794355	-1.380175083	3.282033793	75	H	1.694549575	-2.012190855	2.903252243
76	H	3.918793944	-1.467378519	2.806005394	76	H	4.073063741	-2.014422269	2.296348527
77	C	-6.958750677	1.67692782	-1.571447289	77	C	-6.941400846	1.951675081	-1.52370517
78	C	-7.512990608	2.931125952	-1.776615992	78	C	-7.418766714	3.212450238	-1.862275097

79	C	-7.721762544	0.531271284	-1.645131349	79	C	-7.762095148	0.84500334	-1.49389893
80	C	-8.870832173	3.052690236	-2.055594872	80	C	-8.75942059	3.365937443	-2.190837194
81	C	-9.083187243	0.651592732	-1.890366696	81	C	-9.108168563	1.008332268	-1.804468033
82	C	-9.68434825	1.902314622	-2.085405644	82	C	-9.615560443	2.252947492	-2.164120326
83	O	-9.470238667	4.238708654	-2.322735831	83	O	-9.336503387	4.539350782	-2.541249819
84	O	-11.01719131	1.886914031	-2.338880386	84	O	-10.92413937	2.372165229	-2.52502108
85	O	-9.847727	-0.478094481	-1.888791814	85	O	-9.94164158	-0.068417884	-1.70920516
86	C	-8.707680595	5.426232323	-2.188008707	86	C	-8.510164204	5.678885171	-2.636169735
87	C	-10.27385348	-0.909638108	-3.175773567	87	C	-10.3579779	-0.616431405	-2.953255914
88	C	-11.87467595	2.905043433	-1.826884019	88	C	-11.75984201	2.936682751	-1.523945215
89	H	-6.877819794	3.804685409	-1.731116458	89	H	-6.736633498	4.050990693	-1.873214802
90	H	-7.28844656	-0.448799235	-1.489368018	90	H	-7.39595477	-0.138054323	-1.228154222
91	H	-9.393489979	6.242590179	-2.404420323	91	H	-9.159038514	6.492583091	-2.954412108
92	H	-7.878798735	5.452402752	-2.902244776	92	H	-7.718637439	5.533808222	-3.37972741
93	H	-8.319971241	5.533499982	-1.170076237	93	H	-8.061488157	5.932679646	-1.668829407
94	H	-10.85030071	-1.820841575	-3.021893694	94	H	-10.99335333	-1.468214782	-2.714015827
95	H	-9.409811579	-1.130979263	-3.811655722	95	H	-9.490709776	-0.959521782	-3.527380324
96	H	-10.90235782	-0.155469186	-3.656236788	96	H	-10.92508374	0.116320343	-3.532804915
97	H	-12.8796322	2.489237035	-1.886910405	97	H	-12.77074487	2.93271178	-1.930068009
98	H	-11.81039682	3.820071273	-2.411009198	98	H	-11.46150935	3.964587562	-1.299084462
99	H	-11.63697211	3.124502326	-0.781454426	99	H	-11.730359	2.33304267	-0.611463768
100	C	-7.043252201	-1.772486358	1.464413855	100	C	-6.959395679	-1.929527026	1.488496061
101	C	-7.802757547	-0.626137149	1.495679722	101	C	-7.734585095	-0.809753279	1.691943706
102	C	-7.593720193	-3.035554687	1.643715158	102	C	-7.476561088	-3.216215637	1.582727754
103	C	-9.175186576	-0.73269104	1.71899254	103	C	-9.080511459	-0.977607632	2.012853789
104	C	-8.959544142	-3.140204979	1.871007943	104	C	-8.815070484	-3.381517909	1.913793709
105	C	-9.757779278	-1.983685694	1.911259401	105	C	-9.624184249	-2.254610923	2.133153895
106	O	-9.877890134	0.42730118	1.792508281	106	O	-9.817399162	0.137415156	2.268350753
107	O	-11.09438475	-2.123776799	2.161786346	107	O	-10.9335563	-2.439981082	2.470997823
108	O	-9.61353676	-4.304038451	2.085953962	108	O	-9.425781368	-4.577270961	2.07307801
109	C	-11.4367894	-1.872181459	3.523203617	109	C	-11.18346406	-2.26396703	3.859294274
110	C	-11.09504167	0.536051691	1.050227095	110	C	-10.97972335	0.334136288	1.464103741
111	C	-8.851618494	-5.500492271	2.090373273	111	C	-8.659828861	-5.740691644	1.858808066
112	H	-7.362374879	0.348481081	1.326568597	112	H	-7.329951797	0.190251894	1.60596938
113	H	-6.955252276	-3.906751827	1.603931493	113	H	-6.824548709	-4.060931383	1.410054789
114	H	-12.50477305	-2.064395536	3.618830127	114	H	-12.24267196	-2.468984405	4.013197718
115	H	-11.22488544	-0.832057824	3.793734204	115	H	-10.9554904	-1.238499843	4.168675725
116	H	-10.88280888	-2.542088217	4.187785879	116	H	-10.58826507	-2.966806733	4.451348444
117	H	-11.24366131	1.604339125	0.895077937	117	H	-11.26670847	1.374948481	1.615923643
118	H	-11.94159526	0.132461913	1.609728201	118	H	-11.79444508	-0.325114602	1.771713106
119	H	-11.00573067	0.033730981	0.085275541	119	H	-10.75192602	0.160269035	0.409054809

120	H	-9.559373779	-6.301378106	2.293296294	120	H	-9.335898251	-6.577184956	2.025726792
121	H	-8.088243761	-5.481578861	2.874856867	121	H	-7.822044706	-5.807870355	2.562867124
122	H	-8.376540143	-5.671053862	1.118988741	122	H	-8.275862638	-5.785410396	0.833097109
123	C	6.97081729	1.972736199	1.364328806	123	C	6.935383349	1.677514725	1.725012119
124	C	7.522153279	3.24684754	1.386520518	124	C	7.46457628	2.899270084	2.124174555
125	C	7.734809166	0.845327224	1.571657852	125	C	7.716780819	0.555244436	1.568892663
126	C	8.88397181	3.389700104	1.62957679	126	C	8.825634621	2.986558832	2.386725239
127	C	9.100228502	0.986620874	1.805052314	127	C	9.086126049	0.649410661	1.811924743
128	C	9.688021344	2.254071396	1.838249673	128	C	9.64487661	1.856896452	2.224814021
129	O	9.517282863	4.582391713	1.718839697	129	O	9.455587914	4.104400321	2.81566187
130	O	11.01294217	2.347083925	2.131086693	130	O	10.98155868	1.967861725	2.479425303
131	O	9.802853574	-0.150942974	2.045311475	131	O	9.826026289	-0.481146532	1.674986325
132	C	11.85903436	2.912138781	1.130352583	132	C	11.35199209	1.46060922	3.752882087
133	C	11.02054398	-0.359835741	1.322625912	133	C	10.9757219	-0.413849834	0.830721001
134	C	8.765695949	5.761852308	1.485159051	134	C	8.678405411	5.264403229	3.005932924
135	H	6.885460043	4.103883311	1.218221209	135	H	6.809252695	3.75280445	2.224923325
136	H	7.312816798	-0.14940952	1.531949149	136	H	7.307226324	-0.392646391	1.247134123
137	H	12.86633231	2.554526374	1.343959669	137	H	12.42436663	1.627111933	3.854719036
138	H	11.83143216	4.001200204	1.158408	138	H	11.13642533	0.388786284	3.825670906
139	H	11.55753042	2.559416544	0.137879791	139	H	10.8260828	1.994390018	4.55136311
140	H	11.10817777	-1.435945003	1.172386522	140	H	11.11469369	-1.414062778	0.421866691
141	H	11.8752096	0.010096919	1.890673957	141	H	11.86241511	-0.109952612	1.391686849
142	H	10.97545248	0.130288817	0.34928649	142	H	10.80626491	0.286296419	0.010211223
143	H	9.469980221	6.58530239	1.58233815	143	H	9.367645336	6.031230445	3.354918582
144	H	7.969031462	5.877954628	2.226525927	144	H	7.899043678	5.106026163	3.760600253
145	H	8.335820664	5.765525254	0.478667673	145	H	8.215903367	5.597159621	2.069464422
146	C	11.57600659	-2.894569237	-2.672852668	146	C	11.53603018	-2.265405849	-3.482897634
147	C	8.869223575	-5.595210196	-0.834502878	147	C	8.924158672	-5.236860653	-1.942234648
148	C	6.956941739	-1.88081493	-1.10467926	148	C	6.921058319	-1.570536979	-1.722985184
149	C	7.697751018	-0.748094336	-1.345545575	149	C	7.634433532	-0.398722795	-1.804914547
150	C	7.538822158	-3.141826587	-1.051035839	150	C	7.527469185	-2.812242986	-1.871482706
151	C	9.07424008	-0.859360837	-1.54677799	151	C	9.007134103	-0.453914787	-2.049031608
152	C	8.912916104	-3.250990616	-1.21757312	152	C	8.896882232	-2.868996711	-2.077664919
153	C	9.696507456	-2.10623123	-1.468406099	153	C	9.651925069	-1.684781637	-2.173854867
154	O	9.733878916	0.313415626	-1.730421641	154	O	9.653316559	0.739384728	-2.064418786
155	O	11.05564119	-2.201593948	-1.537274702	155	O	11.01263253	-1.729046195	-2.274499728
156	O	9.59835759	-4.412684956	-1.123199968	156	O	9.606281434	-4.02116726	-2.162292315
157	C	10.7827246	0.392495204	-2.692188537	157	C	10.65776892	0.972124295	-3.039139945
158	H	12.65824267	-2.778918002	-2.630161447	158	H	12.61421023	-2.112085244	-3.441545775
159	H	11.19683572	-2.451804525	-3.599411931	159	H	11.12585815	-1.735595074	-4.350184407
160	H	11.31516886	-3.953406563	-2.63786124	160	H	11.31831416	-3.330807797	-3.569609753

161	H	9.604027156	-6.396271298	-0.79538225	161	H	9.678936145	-6.018578869	-2.004373579
162	H	8.136029117	-5.808948151	-1.618208139	162	H	8.160234964	-5.413568155	-2.70787971
163	H	8.362770824	-5.519775321	0.132738144	163	H	8.459306363	-5.256740675	-0.950683796
164	H	7.252092063	0.236479502	-1.361162551	164	H	7.168636508	0.567999515	-1.669313856
165	H	6.921196817	-4.004766036	-0.846684013	165	H	6.931860805	-3.708992225	-1.780046172
166	H	10.87357299	1.448470367	-2.94444121	166	H	10.73146949	2.054934925	-3.138130312
167	H	10.52387828	-0.169936865	-3.59383624	167	H	10.36829843	0.54390036	-4.004841495
168	H	11.72460453	0.026671245	-2.28319698	168	H	11.61972434	0.562570489	-2.728150639

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