Supporting Information

Macrocyclic Donor–Acceptor Dyads Composed of a Perylene Bisimide Dye Surrounded by Oligothiophene Bridges
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Experimental Section

General Methods

All reactions were performed in standard glass equipment. All used chemicals were purchased from commercial suppliers (*abcr/carbolution chemicals, Acros Organics, Alfa Aesar, Merck, Sigma Aldrich, TCI and VWR*) and applied without further purification. CH$_2$Cl$_2$, THF and toluene were purified and dried with the commercial purification system PureSolv MD from *Innovative Technology*. Preparative column chromatography was performed with self-packed glass columns of several sizes filled with silica gel 60 M (particle size 0.040-0.063 mm, *Merck*). The solvents CH$_2$Cl$_2$ and methanol were freshly distilled prior to use.

Flash column chromatography was performed on a PuriFLash XS-420 from *Interchim* using columns of the sizes 0012, 0025 and 0040. Silica gel deactivation was achieved by flushing the columns with a solvent mixture of cyclohexane/trimethylamine = 20:1 for two column volumes and subsequent purging with pure cyclohexane for five to ten column volumes prior to the actual purification method.

High-resolution MALDI-TOF mass spectra were measured with an ultrafleXtreme mass spectrometer from *Bruker Daltonics GmbH* using trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) as a matrix material. High-resolution ESI-TOF mass spectroscopy was carried out using a microTOF focus instrument from *Bruker Daltonics GmbH*. For melting point measurements an *Olympus BX41* polarisation microscope with a temperature regulator TP84 from *Linkam Scientific* was used. The reported values are uncorrected. The purification by gel permeation chromatography was performed on a *Shimadzu* instrument (LC-20AD Prominence Pump, SPD-MA20A Prominence Diode Array Detector) with two preparative columns (*Japan Analytical Industries Co., Ltd*). Ethanol stabilized CHCl$_3$ (Chromasolv®, *Sigma Aldrich*) was used as eluent.

$^1$H and $^{13}$C NMR spectra were recorded on *Bruker Avance III HD 400* or *600 MHz instruments* using deuterated solvents. $^{13}$C NMR spectra are broad band proton decoupled. Chemical shifts ($\delta$) are listed in parts per million (ppm). Coupling constants ($J$) are stated in Hertz (Hz). The spectra are referenced internally to residual proton
solvent resonances or natural abundance carbon resonances. Multiplicities are reported as s = singlet, brs = broad singlet, d = doublet, dd = doublet of doublets, t = triplet, dt = doublet of triplets, q = quartet, quin = quintet, sex = sextet, m = multiplet with the chemical shift in the center of the signal.

UV/Vis absorption spectra were recorded for solutions in cuvettes (SUPRASIL®, Hellma® Analytics) on a Jasco V-670 or V-770 spectrometer and fluorescence spectra on a FLS980-D2D2-ST fluorescence spectrometer (Edinburgh Instruments) and were corrected against the photomultiplier sensitivity and the lamp intensity.

CV and DPV experiments were carried out with a BASi Epsilon potentiostat connected to a microcell apparatus from rhd instruments involving a 1.6 mL sample container, a platinum counter- and pseudo-reference electrode as well as a glassy carbon working electrode.

Single crystal X-ray diffraction data were collected at the P11 beamline at DESY. The diffraction data were collected by a single 360° scan $\phi$ sweep at 100 K. The diffraction data were indexed, integrated, and scaled using the XDS program package.[S1] In order to compensate low completeness due to single-axis measurement, two data sets were merged using the XPREP program from Bruker.[S2] The structures were solved using SHELXT, expanded with Fourier techniques and refined using the SHELX software package.[S3] Hydrogen atoms were assigned at idealized positions and were included in the calculation of structure factors. All non-hydrogen atoms in the major disorder part of main residues were refined anisotropically. In the crystal structures some of the side chains were disordered and modelled with restraints and constraints using standard SHELX commands RIGU, DELU, ISOR, SADI, SAME, DFIX, DANG, FLAT, SIMU, CHIV and EADP. The solvent molecules in the solvent accessible voids also had disorder and were restrained and/or constrained by a similar set of instructions.

The transient absorption spectrometer setup is based on a femtosecond laser "Solstice" from Newport-Spectra Physics with a fundamental wavelength of 800 nm which provides 100 fs long pulses with a repetition rate of 1 kHz. This laser source was used to pump a NOPA to generate the excitation pulses at 530 nm with a pulse length of around 50 fs. The FWHM-bandwidth of the excitation pulse was 8.5 nm and the pulse energy was set to 20 nJ ((5T)$_2$-PBI) and 15 nJ (5T-PBI). Wire grid polarizers
were used to set the pump pulse polarization to 54.7° in relation to the horizontal polarized white light continuum to achieve magic angle conditions. Another part of the laser beam was guided to a TOPAS-C from Light-Conversion to obtain a wavelength from 1260 nm \((5T)_2\text{-PBI}\) and 1000 nm \(5T\text{-PBI}\) which was used to generate the probing white light continuum within a moving CaF\(_2\) \((5T)_2\text{-PBI}\) or sapphire crystal \(5T\text{-PBI}\). To achieve the probe range from 450 nm to 915 nm a dielectrically coated quartz glass short pass filter with 950 nm, thickness 3 mm, from Edmund-Optics were used. The sample was dissolved in spectroscopic grade dichloromethane from ACROS organics and the solution was filled in a quartz glass cuvette with an optical path length of 0.2 mm \((5T)_2\text{-PBI}\) and 2 mm \(5T\text{-PBI}\). The optical density at the excitation wavelength was set to 0.055 for \((5T)_2\text{-PBI}\) and 0.50 for \(5T\text{-PBI}\). The IRF was ca. 80 fs as measured for stimulated Raman signals of the solvent. Further details on this spectrometer setup are provided in ref\(^{[S4]}\).

Spectroelectrochemical experiments were performed on a Cary 5000 UV/Vis/NIR Spectrometer from Agilent in combination with a sample compartment consisting of a custom-made cylindrical PTFE cell with a sapphire window and an adjustable three in one electrode (6 mm platinum disc working electrode, 1 mm platinum counter and Ag/AgCl leak free reference electrode) in reflection mode. The optical path was adjusted to 100 μm with a micrometer screw. Potentials were applied with a reference potentiostat PAR 283 from Princeton Applied Research. Upon applying a new potential to the solution an equilibration time of 20 seconds between each measurement was employed.

DFT and TD-DFT calculations were performed by Gaussian 16\(^{[S5]}\) using B3LYP/6-31G(d) level of theory.

Stannylated precursor compound \(10\)\(^{[S6]}\) and Ref-PBI\(^{[S7]}\) were synthesized according to literature known procedures. The synthesis of \(5T\) was recently reported.\(^{[S8]}\)
Synthetic Procedure

4-Hexyl-2-(thiophen-2-yl)aniline (2)

A solution of 2-bromo-4-hexylanil ine (3.71 g, 14.5 mmol, 1.00 eq.), 2-thienylboronic acid (5.00 g, 39.1 mmol, 2.70 eq.) and Pd(PPh₃)₂Cl₂ (1.52 g, 2.17 mmol, 15 mol%) in degassed dioxane (50 mL) was stirred for 30 min at room temperature. Subsequently, 20 mL of aqueous K₂CO₃ (1 M) was added and the reaction mixture was refluxed overnight. The suspension was allowed to cool down to room temperature and water (20 mL) was added. The aqueous layer was extracted three times with CH₂Cl₂ (50 mL each) and the combined organic fractions were washed with brine, dried over MgSO₄ and the solvent was removed under reduced pressure. The crude compound was purified by column chromatography (CH₂Cl₂/n-hexane = 1:1) to give compound 2.

Yield: 3.56 g, 13.7 mmol, 95%, yellow oil.

¹H NMR (400 MHz, CD₂Cl₂): δ/ppm = 7.35 (dd, ³J = 5.2 Hz, ⁴J = 1.2 Hz, 1H), 7.20 (dd, ³J = 3.5 Hz, ⁴J = 1.2 Hz, 1H), 7.12 (q, ³J = 3.6 Hz, 1H), 7.08 (dd, ⁴J = 2.1 Hz, ⁵J = 0.4 Hz, 1H), 6.95 (dd, ³J = 8.1 Hz, ⁴J = 2.0 Hz, 1H), 6.69 (d, ³J = 8.1 Hz, 1H), 3.92 (brs, 2H), 2.50 (t, ³J = 7.8 Hz, 2H), 1.60-1.51 (m, 2H), 1.38 - 1.26 (m, 6H), 0.88 (t, ³J = 6.9 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃): δ/ppm = 141.8, 141.5, 133.3, 130.8, 129.1, 127.6, 125.8, 125.2, 120.0, 116.1, 35.1, 31.9, 31.8, 29.1, 22.8, 14.3.

HRMS (ESI-TOF, positive mode, MeCN/CHCl₃ 1:1): m/z calculated for C₁₆H₂₂NS [M+H]⁺: 260.1467, found: 260.1465.

Rf: 0.63 using CH₂Cl₂/n-hexane = 1:1 as eluent.
4-Hexyl-2,6-di(thiophen-2-yl)aniline (3)

A solution of 4-hexylaniline (2.47 g, 7.38 mmol, 1.00 eq.), 2-thienyl boronic acid (2.83 g, 22.1 mmol, 3.00 eq.) and Pd(PPh_3)_2Cl_2 (777 mg, 1.11 mmol, 15 mol%) in degassed dioxane (40 mL) was stirred for 30 min at room temperature. Subsequently, 20 mL of aqueous K_2CO_3 (1 M) was added and the reaction mixture was heated to reflux for three days. The suspension was allowed to cool down to room temperature and water (20 mL) was added. The aqueous layer was extracted three times with CH_2Cl_2 (50 mL each) and the combined organic fractions were washed with brine, dried over MgSO_4 and the solvent was removed under reduced pressure. The crude product was purified by column chromatography (gradient of n-hexane/CH_2Cl_2 = 4:1 to 3:1) to give the title compound 3.

Yield: 1.93 g, 5.67 mmol, 77%, brown oil.

_1H NMR_ (400 MHz, CD_2Cl_2): δ/ppm = 7.38 (dd, 3J = 5.2 Hz, 4J = 1.2 Hz, 2H), 7.24 (dd, 3J = 3.5 Hz, 4J = 1.2 Hz, 2H), 7.14 (dd, 3J = 5.2 Hz, 4J = 3.5 Hz, 2H), 7.08 (s, 2H), 4.28 (brs, 2H), 2.52 (t, 3J = 7.6 Hz, 2H), 1.69 (quin, 3J = 7.3 Hz, 2H), 1.40 - 1.25 (m, 6H), 0.88 (t, 3J = 6.9 Hz, 3H).

_13C NMR_ (101 MHz, CDCl_3): δ/ppm = 141.3, 140.0, 132.5, 131.0, 127.7, 126.3, 125.5, 120.6, 35.0, 31.9, 31.8, 29.2, 22.8, 14.3.

HRMS (ESI-TOF, positive mode, MeCN/CHCl_3 1:1): m/z calculated for C_{20}H_{24}NS_2 [M+H]^+: 342.1345, found: 342.1348.

Rf: 0.46 using CH_2Cl_2/n-hexane = 1:1 as eluent.
N,N'-Di(4-hexyl-2-(thiophen-2-yl)phenyl)-3,4:9,10-tetracarboxylic acid bisimide (4)

A suspension of perylene-3,4:9,10-tetracarboxylic dianhydride (300 mg, 765 μmol, 1.00 eq.), aniline derivate 2 (794 mg, 3.06 mmol, 4.00 eq.) and Zn(OAc)$_2$ (42.0 g, 229 μmol, 0.30 eq) in imidazole (3.0 g, 44.1 mmol) was stirred for 4 h at 120 °C under microwave irradiation. The crude solid was collected with CH$_2$Cl$_2$, adsorbed on celite and the solvent was removed under reduced pressure. The crude product-celite mixture was purified by flash column chromatography (gradient of CH$_2$Cl$_2$/n-hexane = 0:1 to 1:0) to give compound 4.

**Yield**: 492 mg, 562 μmol, 74%, red solid.

**$^1$H NMR** (400 MHz, CD$_2$Cl$_2$): δ/ppm = 8.73 (d, $^3$J = 8.0 Hz, 4H), 8.69 (d, $^3$J = 8.0 Hz, 4H), 7.60 (d, $^4$J = 2.0 Hz, 2H), 7.38 (dd, $^3$J = 8.0 Hz, $^4$J = 2.1 Hz, 2H), 7.26 (d, $^3$J = 7.9 Hz, 2H), 7.15 (dd, $^3$J = 3.6 Hz, $^4$J = 1.2 Hz, 2H), 7.12 (dd, $^3$J = 5.1 Hz, $^4$J = 1.2 Hz, 2H), 6.90 (q, $^3$J = 3.6 Hz, 2H), 2.77 (t, $^3$J = 7.6 Hz, 4H), 1.76 (quin, $^3$J = 7.5 Hz, 4H), 1.41 - 1.34 (m, 12H), 0.93 (t, $^3$J = 7.0 Hz, 6H).

**$^{13}$C NMR** (101 MHz, CDCl$_3$): δ/ppm = 163.9, 144.6, 139.7, 135.1, 133.2, 132.1, 131.0, 130.2, 129.6, 129.3, 127.3, 126.1, 126.0, 123.5, 123.4, 35.9, 31.9, 31.3, 29.3, 22.8, 14.3.

**HRMS** (ESI-TOF, positive mode, MeCN/CHCl$_3$ 1:1): m/z calculated for C$_{56}$H$_{46}$N$_2$NaO$_4$S$_2$ [M+Na]$^+$: 897.2791, found: 897.2736.

**M.p.**: >300 °C.

**R$_f$**: 0.32 using CH$_2$Cl$_2$ as eluent.
**N,N'-Tetra(4-hexyl-2-(thiophen-2-yl)phenyl)-3,4:9,10-tetracarboxylic acid bisimide (5)**

A suspension of perylene-3,4:9,10-tetracarboxylic dianhydride (50.0 mg, 127 μmol, 1.00 eq.), aniline derivate 3 (348 mg, 1.02 mmol, 8.00 eq.) and Zn(OAc)_{2}·2H_{2}O (42.0 mg, 229 μmol, 1.30 eq) in imidazole (600 mg, 8.81 mmol) was stirred for 14 h at 135 °C under microwave irradiation. The crude solid was collected with CH_{2}Cl_{2}, ultrasonicated, adsorbed on celite and the solvent was removed under reduced pressure. The crude product-celite mixture was purified by flash column chromatography (gradient of CH_{2}Cl_{2}/n-hexane = 1:1, CH_{2}Cl_{2}) to give compound 5.

**Yield:** 14.6 mg, 14.1 μmol, 11%, red solid.

**1H NMR** (400 MHz, CD_{2}Cl_{2}): δ/ppm = 8.57 (d, 3J = 8.1 Hz, 4H), 8.69 (d, 3J = 8.1 Hz, 4H), 7.55 (s, 4H), 7.13 (dd, 3J = 3.6 Hz, 4J = 1.1 Hz, 8H), 6.89 (dd, 3J = 3.6 Hz, 4H), 2.80 (t, 3J = 7.8 Hz, 4H), 1.80 (quin, 3J = 7.1 Hz, 4H), 1.50 - 1.35 (m, 12H), 0.93 (t, 3J = 7.0 Hz, 6H).

**13C NMR** (101 MHz, CD_{2}Cl_{2}): δ/ppm = 164.0, 144.9, 139.8, 135.0, 134.6, 132.0, 131.4, 130.0, 129.0, 127.5, 127.0, 126.8, 126.5, 123.5, 123.2, 36.0, 32.1, 31.6, 29.6, 23.0, 14.3.

**HRMS** (MALDI-TOF, positive mode, DCTB in CHCl_{3}): m/z calculated for C_{64}H_{50}N_{2}O_{4}S_{4} [M]^+: 1038.2653, found: 1038.2648.

**M.p.:** >300 °C.

**Rf:** 0.40 using CH_{2}Cl_{2} as eluent.
To a solution of perylene bisimide 4 (480 mg, 549 μmol, 1.00 eq.) in dry THF (100 mL) n-butyllithium (5.14 mL, 1.6 M in n-hexane, 15.0 eq.) was added dropwise under stirring at room temperature and the solution was further stirred for 2 h. Subsequently, Sn(C₄H₉)₃Cl (2.53 mL, 9.32 mmol, 17.0 eq.) was added dropwise at room temperature and the solution was further stirred overnight. The reaction was quenched with water (50 mL), extracted three times with CH₂Cl₂ (50 mL each), and the combined organic layers were washed with brine, dried over MgSO₄ and the solvent was removed under reduced pressure. The crude residue was purified via flash column chromatography (deactivated silica gel, gradient of CH₂Cl₂/n-hexane = 0:1 to 1:0) to give the desired compound 6.

**Yield:** 355 mg, 244 μmol, 45%, deep red solid.

**¹H NMR** (400 MHz, CD₂Cl₂): δ/ppm = 8.73 (d, ³J = 8.0 Hz, 4H), 8.69 (d, ³J = 8.0 Hz, 4H), 7.52 (d, ⁴J = 2.0 Hz, 2H), 7.38 (dd, ³J = 8.0 Hz, ⁴J = 2.1 Hz, 2H), 7.32 (d, ³J = 3.5 Hz, 2H), 1.77 (quin, ³J = 7.8 Hz, 4H), 1.42 - 1.35 (m, 12H), 1.04 (sex, ³J = 7.4 Hz, 12H), 0.93 (t, ³J = 7.0 Hz, 6H), 0.80 (t, ³J = 8.1 Hz, 12H), 0.64 (t, ³J = 7.4 Hz, 18H).

**¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 164.0, 145.3, 144.9, 138.4, 135.8, 135.1, 133.5, 131.8, 130.3 (2 signals), 130.0, 128.9, 127.4, 126.8, 123.8, 123.7, 36.1, 32.2, 31.7, 29.6, 29.0, 27.4, 23.1, 14.3, 13.6, 10.9.

**HRMS** (ESI-TOF, positive mode, MeCN/CHCl₃ 1:1): m/z calculated C₆₀H₆₈N₂NaO₄S₂Sn₂ [M+Na]⁺: 1477.4904, found: 1477.4821.

**M.p.:** 116-118 °C.

**Rr:** 0.55 using CH₂Cl₂ as eluent.
$N,N'$-Tetra(4-hexyl-2-(5-(tributylstannyl)thiophen-2-yl)phenyl)-3,4:9,10-tetracarboxylic acid bisimide (7)

To a solution of perylene bisimide 5 (108 mg, 104 μmol, 1.00 eq.) in dry THF (22 mL) $n$-butyllithium (1.30 mL, 1.6 M in $n$-hexane, 20.0 eq.) was added dropwise under stirring at room temperature and the solution was further stirred for 1 h. Subsequently, Sn(C$_4$H$_9$)$_3$Cl (676 μL, 2.49 mmol, 24.0 eq.) was added dropwise at room temperature and the solution was further stirred overnight. The reaction was quenched with water (15 mL), extracted three times with CH$_2$Cl$_2$ (50 mL each), and the combined organic layers were washed with brine, dried over MgSO$_4$ and the solvent was removed under reduced pressure. The crude residue was purified via flash column chromatography (deactivated silica gel, gradient of $n$-hexane/ CH$_2$Cl$_2$ = 1:0 to 1:1) to yield the desired compound 7.

**Yield**: 45.1 mg, 20.5 μmol, 20%, deep red solid.

$^1$H NMR (400 MHz, CD$_2$Cl$_2$): $\delta$/ppm = 8.65 (d, $^3$J = 7.9 Hz, 4H), 8.62 (d, $^3$J = 7.9 Hz, 4H), 7.55 (s, 4H), 7.27 (d, $^3$J = 3.4 Hz, 4H), 6.94 (d, $^3$J = 3.4 Hz, 4H), 2.79 (t, $^3$J = 7.7 Hz, 4H), 1.79 (quin, $^3$J = 7.2 Hz, 4H), 1.52-1.46 (m, 4H), 1.41-1.36 (m, 8H), 1.32 - 1.24 (m, 24H), 1.06 (sex, $^3$J = 7.4 Hz, 24H), 0.93 (t, $^3$J = 7.0 Hz, 6H), 0.82 (t, $^3$J = 8.1 Hz, 24H), 0.67 (t, $^3$J = 7.2 Hz, 36H).

$^{13}$C NMR (150 MHz, CD$_2$Cl$_2$): $\delta$/ppm = 164.2, 145.3, 144.8, 138.5, 135.7, 135.3, 134.8, 132.1, 130.2, 130.1, 128.1, 127.9, 127.0, 123.8, 123.6, 36.1, 32.2, 31.6, 29.7, 29.0, 27.4, 23.0, 14.3, 13.7, 11.0.

HRMS (MALDI-TOF, positive mode, DCTB in CHCl$_3$): m/z calculated C$_{112}$H$_{154}$N$_2$NaO$_4$S$_4$Sn$_4$ [M+Na]$^+$: 2221.6772, found: 2221.6771.

M.p.: 183-185 °C.

R: 0.73 using CH$_2$Cl$_2$/cyclohexane = 2:1 as eluent.
N,N'-Di(4-hexyl-2-(5-chloro(1,5-cyclooctadiene)platinum)thiophen-2-yl)phenyl)-3,4:9,10-tetracarboxylic acid bisimide (8)

A solution of 6 (50.0 mg, 34.4 μmol, 1.0 eq.) and Pt(COD)Cl$_2$ (28.3 mg, 75.5 μmol, 2.2 eq.) in degassed toluene (10 mL) was stirred for 2 h at 95 °C. The solvent was removed under reduced pressure and the crude product was purified via flash column chromatography (gradient of CH$_2$Cl$_2$/acetone = 1:0 to 20:1) to yield compound 8.

**Yield:** 31.0 mg, 20.0 μmol, 58%, deep red solid.

**$^1$H NMR (400 MHz, C$_2$D$_2$Cl$_4$):** δ/ppm = 8.70 (brs, 8H), 7.59 (d, $^3$J = 1.9 Hz, 2H), 7.32 (dd, $^3$J = 1.9 Hz, $^3$J = 8.0 Hz, 2H), 7.24 ($^3$J = 8.0 Hz), 7.08 (d, $^3$J = 3.7 Hz, 2H), 6.77 (d, $^3$J = 3.7 Hz, 2H), 5.60-5.52 (m, 4H), 4.96-4.89 (m, 4H), 2.75 (t, $^3$J = 7.7 Hz, 4H), 2.47-2.12 (m, 16H), 1.74 (quin, $^3$J = 7.3 Hz, 4H), 1.38-1.26 (m, 12H), 0.93 (t, $^3$J = 7.0 Hz, 6H).

**$^{13}$C NMR (101 MHz, C$_2$D$_2$Cl$_4$):** δ/ppm = 163.6, 144.3, 141.1, 138.5, 134.7, 133.3, 131.9, 130.3, 129.7, 129.4, 129.2, 128.1, 126.3, 126.0, 123.2, 120.2, 112.9, 90.1, 35.7, 31.6, 31.5, 31.2, 30.8, 29.1, 28.3, 22.6, 14.2.

**HRMS (MALDI-TOF, positive mode, DCTB in CHCl$_3$):** m/z calculated for C$_{72}$H$_{68}$Cl$_2$N$_2$O$_4$Pt$_2$S$_4$ [M]$^+$: 1548.3293, found: 1548.3288.

**M.p.:** >300 °C.

**Rf:** 0.29 using CH$_2$Cl$_2$/acetone = 20:1 as eluent.
A solution of 7 (49.6 mg, 22.6 μmol, 1.0 eq.) and Pt(cod)Cl₂ (169 mg, 452 μmol, 20.0 eq.) in degassed toluene (25 mL) was stirred overnight at 80 °C. The solvent was removed under reduced pressure and the crude product was purified via flash column chromatography (gradient of CH₂Cl₂/MeOH = 1:0 to 99:1) to yield compound 9.

**Yield**: 44.4 mg, 217 μmol, 82%, deep red solid.

**¹H NMR** (400 MHz, C₂D₂Cl₄): \( \delta / \text{ppm} = 8.66 \) (brs, 8H), 7.48 (brs, 4H), 7.10 (brs, 4H), 6.77 (brs, 4H), 5.55 (brs, 8H), 4.85 (brs, 8H), 2.77-2.70 (m, 4H), 2.44-2.36 (m, 8H), 2.32-2.24 (m, 4H), 2.15-2.10 (m, 4H), 1.78-1.71 (m, 4H), 1.39-1.34 (m, 12H), 0.96-0.91 (m, 6H).

**¹³C NMR** (150 MHz, C₂D₂Cl₄): \( \delta / \text{ppm} = 163.7, 141.2, 138.4, 134.5, 134.2, 132.1, 130.2, 126.5, 123.4, 120.2, 116.7, 116.5, 116.3, 112.9, 100.3, 99.4, 90.0, 35.7, 31.5, 30.8, 29.6, 29.2, 28.3, 22.6, 14.2.

**HRMS** (MALDI-TOF, positive mode, DCTB in CHCl₃): \( m/z \) calculated C₉₆H₉₄Cl₄N₂O₄Pt₄S₄ [M]+: 2386.3441, found: 2386.3437.

**M.p.**: >300 °C.

**Rf**: 0.44 using CH₂Cl₂/MeOH = 20:1 as eluent.
To a stirred solution of 8 (31.0 mg, 20.0 μmol, 1.00 eq.) in degassed toluene (40 mL) was added dropwise the stannylated oligothiophene 10 (21.9 mg, 37.8 μmol, 1.10 eq.) in degassed toluene (1.0 mL) via a syringe pump over 15 h and the reaction mixture was stirred overnight at 75 °C. The solvent was removed in vacuo and the crude residue was washed with n-hexane. The crude product was redissolved in degassed CH₂Cl₂ (40 mL) and 1,1'-bis(diphenylphosphino)ferrocene (24.4 mg, 75.5 μmol, 2.20 eq.) was added. The solution was stirred for 6 h at room temperature. The solvent was removed in vacuo and the residue was dissolved in degassed m-xylene (40 mL) and stirred overnight at 120 °C. The solvent was removed under reduced pressure and the crude product was purified via flash column chromatography (CH₂Cl₂/cyclohexane = 1:1 to 1:0) and gel permeation chromatography (CHCl₃) to give the desired compound.

**Yield**: 7.71 mg, 5.99 μmol, 30%, red orange solid.

**¹H NMR** (600 MHz, CD₂Cl₂): δ/ppm = 8.70 (s, 8H), 7.79 (d, 4J = 1.8 Hz, 2H), 7.45 (d, 3J = 4.0 Hz, 2H), 7.36 (dd, 3J = 8.0 Hz, 4J = 1.8 Hz, 2H), 7.30 (d, 3J = 8.0 Hz, 2H), 7.19 (d, 3J = 4.0 Hz, 2H), 7.03 (s, 2H), 6.88 (s, 2H), 2.80 (t, 3J = 7.7 Hz, 4H), 2.58 (t, 3J = 7.9 Hz, 4H), 1.79 (quin, 3J = 7.6 Hz, 4H), 1.35-1.42 (m, 8H), 1.22-1.31 (m, 20H), 0.94 (t, 3J = 7.0 Hz, 6H), 0.83 (t, 3J = 7.0 Hz 6H).

**¹³C NMR** (150 MHz, CD₂Cl₂): δ/ppm = 164.2, 145.0, 141.5, 138.1, 137.8, 135.7, 135.5, 135.1, 132.2, 132.0, 130.7, 130.1, 129.5, 129.3, 129.2, 128.6, 127.7, 127.0, 126.9, 126.8, 124.1, 123.8, 123.6, 36.2, 32.2, 32.0, 31.7, 30.7, 29.6, 29.5, 23.1, 22.9, 14.3, 14.2.

**HRMS** (MALDI-TOF, positive mode, DCTB in CHCl₃): m/z calculated C₈₀H₇₄N₂O₄S₅ [M]+: 1286.4252, found: 1286.4247.

**UV/Vis** \(λ_{\text{max}}\) (ε\(\text{max}\)): CH₂Cl₂: 531 nm (64.8 × 10³ L mol⁻¹ cm⁻¹).

**Fluorescence** \(λ_{\text{max}}\) (λ\(\text{ex}\)): Cyclohexane: 528 nm (480 nm). \(Φ_{\text{f}}\) = < 0.1%.

**Rf**: 0.32 using CH₂Cl₂ as eluent.
To a stirred solution of 9 (44.4 mg, 18.5 μmol, 1.00 eq.) in degassed toluene (25 mL) was added dropwise the stannylated oligothiophene 10 (40.7 mg, 40.9 μmol, 2.20 eq.) in degassed toluene (1.0 mL) via a syringe pump over 15 h and the reaction mixture was stirred overnight at 75 °C. The solvent was removed in vacuo and the crude residue was washed with n-hexane. The crude product was redissolved in degassed CH2Cl2 (25 mL) and 1,1’-bis(diphenylphosphino)ferrocene (45.3 mg, 81.7 μmol, 4.40 eq.) was added. The solution was stirred for 6 h at room temperature. The solvent was removed in vacuo and the residue was dissolved in degassed m-xylene (25 mL) and stirred overnight at 120 °C. The solvent was removed under reduced pressure and the crude product was purified via flash column chromatography (cyclohexane / CH2Cl2 = 1:0 to 1:1) and gel permeation chromatography (CHCl3) to give the desired compound.

**Yield:** 1.26 mg, 676 nmol, 4%, red orange solid.

**1H NMR** (400 MHz, CD2Cl2): δ/ppm = 8.84 (d, 3J = 8.4 Hz, 4H), 8.74 (d, 3J = 7.9 Hz, 4H), 7.73 (s, 4H), 7.43 (d, 3J = 3.9 Hz, 4H), 7.20 (d, 3J = 3.9 Hz, 4H), 7.04 (s, 4H), 6.90 (s, 4H), 2.85 (t, 3J = 7.8 Hz, 4H), 2.60 (t, 3J = 7.6 Hz, 8H), 1.84 (quin, 3J = 7.3 Hz, 4H), 1.50-1.27 (m, 44H), 0.95 (t, 3J = 7.1 Hz, 6H), 0.88 (t, 3J = 6.7 Hz, 12H).

**13C NMR** (150 MHz, CD2Cl2): δ/ppm = 164.6, 145.1, 141.3, 138.3, 138.1, 135.9, 135.7, 134.0, 132.3, 130.3, 129.7, 129.2, 128.9, 127.2, 127.1, 126.5, 125.8, 124.5, 123.8, 123.7, 36.2, 32.2, 32.0, 31.6, 30.7, 30.1, 29.7, 29.5, 23.1, 23.0, 14.3, 14.2.

**HRMS** (MALDI-TOF, positive mode, DCTB in CHCl3): m/z calculated for C112H106N2O4S10 [M+H]+: 1862.5360, found: 1862.5354.

**UV/Vis** λmax (εmax): CH2Cl2: 380 nm (93.9 × 10³ L mol⁻¹ cm⁻¹).

**Fluorescence** λmax (λex): Cyclohexane: 528 nm (480 nm). Φf = <0.1%

**Rf:** 0.81 using CH2Cl2/cyclohexane = 2:1 as eluent.
Figure S1. Aromatic region of the $^1$H NMR spectra (400 MHz) of Ref-PBI, 5T, 5T-PBI and (5T)$_2$-PBI (from bottom to top) in CD$_2$Cl$_2$ at 298 K.
## Single Crystal X-ray Analysis

**Table S1.** Crystal data and structure refinement for (5T)$_2$-PBI

| Property                                      | Value                                      |
|-----------------------------------------------|--------------------------------------------|
| CCDC Number                                   | 2102595                                    |
| Empirical formula                             | C$_{120.64}$H$_{113.21}$Cl$_{1.44}$N$_2$O$_4$S$_{10}$ |
| Formula weight                                | 2026.55                                    |
| Temperature                                   | 100(2) K                                   |
| Wavelength                                    | 0.61992 Å                                  |
| Crystal system                                | Triclinic                                   |
| Space group                                   | P-1                                        |
| Unit cell dimensions                          |                                            |
| \( a \)                                       | 15.385(10) Å                               |
| \( \alpha \)                                  | 74.973(5)°                                 |
| \( b \)                                       | 17.342(3) Å                                |
| \( \beta \)                                   | 89.82(2)°                                 |
| \( c \)                                       | 31.216(5) Å                                |
| \( y \)                                       | 85.158(16)°                                |
| Volume                                        | 8014(5) Å\(^3\)                           |
| \( Z \)                                       | 3                                          |
| Density (calculated)                          | 1.260 mg/m\(^3\)                          |
| Absorption coefficient                        | 0.203 mm\(^{-1}\)                        |
| \( F(000) \)                                  | 3202.4                                     |
| Crystal size                                  | 0.100 x 0.100 x 0.100 mm\(^3\)             |
| Theta range for data collection               | 0.589 to 27.653°                           |
| Index ranges                                  | 22 ≤ \( h \) ≤ 22, 25 ≤ \( k \) ≤ 24, 45 ≤ \( l \) ≤ 46 |
| Reflections collected                         | 264918                                     |
| Independent reflections                       | 43791 \([R_{\text{int}} = 0.0914]\)        |
| Completeness to theta = 21.836°               | 98.8\%                                     |
| Absorption correction                         | None                                       |
| Refinement method                             | Full-matrix least-squares on \( F^2 \)    |
| Data / restraints / parameters                 | 43791 / 4155 / 2852                        |
| Goodness-of-fit on \( F^2 \)                  | 1.109                                      |
| Final R indices \([I > 2\sigma(I)]\)          | \( R_1 = 0.0848, wR_2 = 0.2698 \)         |
| R indices (all data)                           | \( R_1 = 0.1117, wR_2 = 0.3036 \)         |
| Extinction coefficient                         | n/a                                        |
| Largest diff. peak and hole                    | 0.624 and −0.664 e·Å\(^{-3}\)             |
Figure S2. a) Front view of a single (5T)$_2$-PBI centrosymmetric molecule A (ORTEP drawing in 50% probability for thermal ellipsoids). PBI chromophore is coloured in red, macrocycle in blue and solubilizing alkyl chains in grey. Crystal packing seen approximately along the a-, c-, and b-axes for b), c) and d), respectively. Heavily disordered aliphatic chains as well as solvent molecules were omitted for clarity.

Figure S3. a) Front, b) side and c) top view onto the unsymmetric molecule B of (5T)$_2$-PBI. Heavily disordered aliphatic chains as well as solvent molecules were omitted for clarity. d) Unit cell including all structural disorder (violet) and aliphatic chains (grey). The ellipsoids are set to 50% probability.
DFT Calculations

Rotational Barrier:
To estimate the rotational barrier (Figure S4) of the imide substituent of 8, calculations were conducted only on one half-segment, namely the naphthalene imide part (Figure S4b). In order to estimate the energy cost of this rotation a dihedral angle scan of $\alpha$ in 0.5° intervals was performed (Figure S4a). Here, the change of the total energies $\Delta E$ depending on the torsion angle $\alpha$ is plotted. This angle $\alpha$, which was modified during the scan, is highlighted in Figure S4c. The initial $\alpha$ of 90° between the phenyl substituent and the naphthalene monoimide core was readily reduced until complete rotation of the substituent. In the starting geometry (Figure S4c) the sulphur atom points away from the naphthalene imide core, whereas during the rotation this subunit undergoes a conformational change at $\alpha = 59°$ (Figure S4d) towards the core due to the repulsive hydrogen-core interaction. Further rotation up to $-26°$ leads to an outer plane uplifting of the nitrogen atom (Figure S4e) and an almost perpendicular angle between the thiophene and the phenyl group. This geometry also resembles the structure with the highest total energy level during the entire rotation process and therefore the closest structure to the "real" transition state (TS). This geometry was the basis for the TS calculation of which the result is shown in Figure S4f. The energy difference between this TS geometry and the fully relaxed monoimide is 114 kJ mol$^{-1}$ and can therefore be considered as the rotational barrier or the Gibbs free energy of activation $\Delta G^\ddagger$. To determine the half life time of the rotation event the reaction rate $k_{rot}$ according to Eyring has to be determined first (Eq. 1)

$$k_{rot} = \frac{k_B T}{h} \cdot e^{-\frac{\Delta G^\ddagger}{RT}}.$$  \hspace{1cm} (1)

Here $k_B$ is the Boltzmann constant, $T$ the temperature $R$ and $h$ the Planck constant. For $T = 298.15$ K (room temperature) and 348.15 K (macrocyclization reaction temperature) the resulting $k_{rot}$ values are $6.60 \cdot 10^{-8}$ s$^{-1}$ and $5.70 \cdot 10^{-5}$ s$^{-1}$, respectively. The half life time $t_{1/2}$ (Eq. 2) can be calculated by the following equation:

$$t_{1/2} = \frac{ln(2)}{4 k_{rot}}.$$ \hspace{1cm} (2)

The results of $t_{1/2} = 30$ days at room temperature (25 °C) and around 51 min at 75 °C show the importance of elevated temperatures during the final macrocyclization reaction towards 5T-PBI.$^{[S9]}$
Figure S4. a) Plot of the change in total energy $\Delta E$ against the dihedral angle $\alpha$. b) Chemical structure of the molecular fragment used for the calculations. c) Geometry optimized structure of the starting geometry for the rotational scan and the starting angle $\alpha$ incorporated by the planes of the naphthalene (red) and phenylene (blue) subunit. d) Geometry with $\alpha = 59^\circ$. e) Highest energy geometry with $\alpha = -26^\circ$. f) Geometry of the TS. All calculations were conducted with DFT at the B3LYP/6-31G(d) level of theory.

Figure S5. Side view (a), view along the $N,N'$-axis (b) and top view (c) onto the PBI $\pi$-surface of geometry optimized structures of 5T-PBI and (5T)$_2$-PBI (from top to bottom). The quantum mechanics calculations were carried out on the level of B3LYP density functional with the 6-31G(d) basis set as implemented in with Gaussian 16. Aliphatic chains were replaced by methyl groups. Color code: carbon = light grey, hydrogen = white, nitrogen = blue, oxygen = red, sulfur = yellow.

Strain energies:
The strain energies of the macrocycles (5T)$_2$-PBI and 5T-PBI were calculated as follows: The connecting C-C bonds between two thiophene units of the bridges were removed virtually from the optimized geometries of (5T)$_2$-PBI and 5T-PBI and the obtained radicals were saturated by thiophene capping molecules to retain the local
environment of the two ends. Geometry optimization leads to the lowest energy conformation of the resulting structures and complete macrocyclic induced strain release of both subunits. Figure S6 shows the optimized geometries of these open macrocycles 11 and 12 as well as capping bithiophene 13.

![Figure S6](image)

**Figure S6.** Front view of the optimized geometries of the non-cyclic structures 11 and 12 as well as bithiophene 13. The quantum mechanics calculations were carried out on the level of B3LYP density functional with the 6-31G(d) basis set as implemented in with Gaussian 16. Aliphatic chains were replaced by methyl groups. Color code: carbon = light grey, hydrogen = white, nitrogen = blue, oxygen = red, sulfur = yellow.

The strain energies of the respective macrocycles (\(E_{\text{Strain}}\)) were determined by comparing the lowest energy conformation of the respective macrocycles (\(E_{\text{5T-PBI}}\) or \(E_{(5T)_2-PBI}\)) to the homodesmic reaction product\(^{[S10]}\) of the linear structures 11 and 12 (\(E_{11}\) or \(E_{12}\)) and the bithiophene cap 13 (\(E_{13}\)):

\[
E_{\text{Strain}, (5T)_2-PBI} = (E_{5T2-PBI} + 2E_{13}) - E_{11} = 30.6 \text{ kJ mol}^{-1} \quad (3)
\]

\[
E_{\text{Strain}, 5T-PBI} = (E_{5T-PBI} + E_{13}) - E_{12} = 13.9 \text{ kJ mol}^{-1} \quad (4)
\]

**Table S2:** First excited state (S1) energy predictions of 5T-PBI and (5T)_2-PBI with TDDFT at the B3LYP/6-31G(d) level of theory (H = HOMO, L = LUMO).

| Compound   | Excitation Energy / eV | Wavelength / nm | Osc. Strength | Contribution       |
|------------|------------------------|-----------------|---------------|--------------------|
| 5T-PBI     | 1.18                   | 1051            | 0.0000        | H → L (100%)       |
| (5T)_2-PBI | 1.32                   | 937             | 0.0001        | H → L (100%)       |
**Electrochemistry**

**Figure S7** Cyclic voltammogram (solid line) initiated in the forward (positive-going) scan direction (marked by an arrow) at a scan rate of 100 mV s\(^{-1}\) and differential pulse voltammogram (dashed line) of **Ref-PBI** in CH\(_2\)Cl\(_2\) with Bu\(_4\)NPF\(_6\) at room temperature (c\(_0\) = 10\(^{-4}\) M).

In order to demonstrate the involvement of four electrons in the entire oxidation process of (5T\(_2\)-PBI we decided to utilize the baseline (recorded prior to the actual measurement) corrected DPV data which was compared to those of 5T-PBI. It is evident that for respective reduction of both macrocyclic PBI subunits two electrons are transferred. By comparing the PBI’s DPV reduction to the oligothiophene’s oxidation wave integrals the relative amount of transported charges can be assigned (Figure S8).

**Figure S8.** DPV measurements of a) (5T\(_2\)-PBI and b) 5T-PBI in CH\(_2\)Cl\(_2\) solutions with Bu\(_4\)NPF\(_6\) at room temperature (c\(_0\) = 10\(^{-4}\) M). The wave integrals for PBI reduction and oligothiophene oxidation are highlighted in red and blue, respectively. The straight black lines mark the integration limits and the values above the waves represent the absolute integral in arbitrary units. The graphs are baseline corrected to ease the integration.
The ratio of both signals in reduction and oxidation determined by integration for 5T-PBI is 1.62/1.59 = 1.02 ≈ 1 and for (5T)₂-PBI 3.41/1.56 = 2.19 ≈ 2, respectively. The ratios prove that approximately double the amount of charges was transferred in the oxidation process of (5T)₂-PBI in comparison to the reduction. For 5T-PBI an equal amount of charges are involved in reduction and oxidation.

**Molecular Orbital DFT Calculations**

![Figure S9. a) LUMO and b) HOMO of 5T-PBI based on geometry optimized structures from DFT calculations. The quantum mechanics calculations were carried out on the level of B3LYP density functional with the 6-31G(d) basis set as implemented in with Gaussian 16.](image)

**Spectroscopy in CH₂Cl₂**

![Figure S10. Normalized UV/Vis spectra (black lines) and emission spectra with the excitation wavelengths λₑₓ = 400 nm (maroon lines) and λₑₓ = 480 nm (red lines) of a) a 1:1 mixture of Ref-PBI + 5T, b) 5T-PBI and c) (5T)₂-PBI. All UV/Vis and emission (c₀ = 10⁻⁷ M) measurements were carried out in CH₂Cl₂ at room temperature. d) Photograph of Ref-PBI, 5T, 5T-PBI and (5T)₂-PBI (from left to right) in CH₂Cl₂ under 365 nm UV light irradiation.](image)
Spectroscopy in Cyclohexane

Figure S11. Normalized UV/Vis absorption (black solid) and emission (red: $\lambda_{ex} = 480$ nm, maroon: $\lambda_{ex} = 340/310$ nm) spectra of 5T-PBI (bottom) and (5T)$_2$-PBI (top) in cyclohexane at room temperature ($c_0 = 10^{-7}$ M). The wavelengths for excitation to obtain the fluorescence spectra are highlighted by arrows.

Table S3. Spectroscopic properties of 5T-PBI and (5T)$_2$-PBI in cyclohexane at room temperature.

|          | $\lambda_{abs,max}$ \[^a\] / nm | $\lambda_{em,max}$ \[^a,\^[b]\] / nm | $\lambda_{em,max}$ \[^a,\^[c]\] / nm | $\Delta\bar{\nu}_{\text{Stokes}}$ (PBI) \[^a\] / cm$^{-1}$ | $\Phi_{\text{fl}}$ \[^a,\^[d]\] / % |
|----------|-------------------------------|-------------------------------|-------------------------------|---------------------------------|---------------------------------|
| 5T-PBI   | 519                           | 531                           | 528                           | 329                             | << 0.1                          |
| (5T)$_2$-PBI | 374                      | 536                           | 528                           | 145                             | << 0.1                          |

[^a]: $c_0 = 10^{-7}$ M. \[^b\]: $\lambda_{ex} = 340/310$ nm. \[^c\]: $\lambda_{ex} = 480$ nm \[^d\]: The fluorescence quantum yields of the PBI were measured relative to $N,N'$-bis(2,6-diisopropylphenyl)-1,6,7,12-tetraphenoxy-perylenebis(dicarboximide) \[^51\] (96% in CHCl$_3$) as a reference at four different excitation wavelengths in the spectral region of the PBI absorption band.

Transient Absorption

Figure S12. a) Transient absorption spectra of 5T-PBI in CH$_2$Cl$_2$ after excitation at 530 nm and b) time scans and fit (red line) at selected wavelengths.
Figure S13. a) Transient absorption spectra of (5T)\textsubscript{2}-PBI in CH\textsubscript{2}Cl\textsubscript{2} after excitation at 530 nm and b) time scans and fit (red line) at selected wavelengths.

Figure S14. a) Normalized UV/Vis/NIR absorption spectra of 5T-PBI (black line) upon electrochemical reduction to 5T-PBI\textsuperscript{•−} (red line) and electrochemical oxidation to 5T\textsuperscript{•+}-PBI (blue line) in CH\textsubscript{2}Cl\textsubscript{2} solutions with Bu\textsubscript{4}NPF\textsubscript{6} at room temperature (c\textsubscript{0} = 10\textsuperscript{−4} M). b) Evolution associated difference spectra (EADS) and lifetimes from a global fit analysis of the transient spectra of 5T-PBI obtained by excitation at 530 nm in CH\textsubscript{2}Cl\textsubscript{2} (c\textsubscript{0} = 10\textsuperscript{−4} M) at room temperature.
NMR Spectra

Figure S15. $^1$H NMR spectrum of 2 in CD$_2$Cl$_2$ at 298 K.

Figure S16. $^{13}$C NMR spectrum of 2 in CDCl$_3$ at 298 K.
Figure S17. $^1$H NMR spectrum of 3 in CD$_2$Cl$_2$ at 298 K.

Figure S18. $^{13}$C NMR spectrum of 3 in CDCl$_3$ at 298 K.
Figure S19. $^1$H NMR spectrum of 4 in CD$_2$Cl$_2$ at 298 K.

Figure S20. $^{13}$C NMR spectrum of 4 in CDCl$_3$ at 298 K.
Figure S21. $^1$H NMR spectrum of 5 in CD$_2$Cl$_2$ at 298 K.

Figure S22. $^{13}$C NMR spectrum of 5 in CD$_2$Cl$_2$ at 298 K.
Figure S23. $^1$H NMR spectrum of 6 in CD$_2$Cl$_2$ at 298 K.

Figure S24. $^{13}$C NMR spectrum of 6 in CD$_2$Cl$_2$ at 298 K.
Figure S25. $^1$H NMR spectrum of 7 in CD$_2$Cl$_2$ at 298 K.

Figure S26. $^{13}$C NMR spectrum of 7 in CD$_2$Cl$_2$ at 298 K.
Figure S27. $^1$H NMR spectrum of 8 in C$_2$D$_2$Cl$_4$ at 298 K.

Figure S28. $^{13}$H NMR spectrum of 8 in C$_2$D$_2$Cl$_4$ at 298 K.
Figure S29. $^1$H NMR spectrum of 9 in C$_2$D$_2$Cl$_4$ at 298 K.

Figure S30. $^{13}$C NMR spectrum of 9 in C$_2$D$_2$Cl$_4$ at 298 K. Residual signals of CHCl$_3$ (79.5 ppm), H-grease (31.1 pm) and cyclohexane (26.8 ppm).
Figure S31. $^1$H NMR spectrum of 5T-PBI in CD$_2$Cl$_2$ at 298 K.

Figure S32. $^{13}$C NMR spectrum of 5T-PBI in CD$_2$Cl$_2$ at 298 K.
Figure S33. $^1$H NMR spectrum of (5T)$_2$-PBI in CD$_2$Cl$_2$ at 298 K.

Figure S34. $^{13}$C NMR spectrum of (5T)$_2$-PBI in CD$_2$Cl$_2$ at 298 K.
Mass Spectra

Figure S35. HRMS (ESI-TOF, pos. mode, acetonitrile/chloroform 1/1) spectra of 2.

Figure S36. HRMS (ESI-TOF, pos. mode, acetonitrile/chloroform 1/1) spectra of 3.

Figure S37. HRMS (ESI-TOF, pos. mode, acetonitrile/chloroform 1/1) spectra of 4.
Figure S38. HRMS (MALDI-TOF, pos. mode, DCTB in CHCl₃) spectra of 5.

Figure S39. HRMS (MALDI-TOF, pos. mode, DCTB in CHCl₃) spectra of 6.
Figure S40. HRMS (MALDI-TOF, pos. mode, DCTB in CHCl₃) spectra of 7.

Figure S41. HRMS (MALDI-TOF, pos. mode, DCTB in CHCl₃) spectra of 8.
Figure S42. HRMS (MALDI-TOF, pos. mode, DCTB in CHCl₃) spectra of 9.

Figure S43. HRMS (MALDI-TOF, pos. mode, DCTB in CHCl₃) spectra of 5T-PBI.
Figure S44. HRMS (MALDI-TOF, pos. mode, DCTB in CHCl₃) spectra of (5T)₂-PBI.
Cartesian Coordinates Received from DFT Calculations

Final geometry:

Total energy: $-4708.34654570$ Hartrees

| Atom | X    | Y    | Z    | Coordinates |
|------|------|------|------|-------------|
| C1   | 3.0379300 | -2.5972200 | 2.2171600 |
| C2   | 1.6430100 | -2.5910200 | 2.3218800 |
| C3   | 0.8187400 | -2.5326100 | 1.1964300 |
| C4   | 1.4289000 | -2.5046600 | -0.0976600 |
| C5   | 2.8550800 | -2.4869600 | -0.1948300 |
| C6   | 3.6491100 | -2.5346100 | 0.9767800 |
| C7   | 0.6476300 | -2.4889500 | -1.2965900 |
| C8   | 1.3097700 | -2.4262600 | -2.5242200 |
| C9   | 2.7053000 | -2.3863200 | -2.6099900 |
| C10  | 3.4804400 | -2.4197700 | -1.4635800 |
| C11  | 5.1297100 | -2.5217600 | 0.9018100 |
| C12  | 4.9560900 | -2.3587000 | -1.5897800 |
| C13  | -0.6476200 | -2.4888000 | 1.2968900 |
| C14  | -0.8187400 | -2.5327500 | -1.1961300 |
| C15  | -1.4288900 | -2.5046500 | 0.0979600 |
| C16  | -2.8550700 | -2.4869400 | 0.1951300 |
| C17  | -3.6491100 | -2.5347200 | -0.9764800 |
| C18  | -3.0379300 | -2.5974800 | -2.1685000 |
| C19  | -1.6430100 | -2.5912900 | -2.3215700 |
| C20  | -1.3097700 | -2.4259700 | 2.5245100 |
| C21  | -2.7053000 | -2.3860100 | 2.6102800 |
| C22  | -3.4804400 | -2.4196000 | 1.4638700 |
| C23  | -4.9560900 | -2.3582000 | 1.5900700 |
| C24  | -5.1297000 | -2.5218700 | -0.9015100 |
| N25  | 5.6928700 | -2.3926100 | -0.3869500 |
| N26  | -5.6928700 | -2.3925600 | 0.3872300 |
| O27  | -5.8410700 | -2.6076100 | -1.8887600 |
| O28  | -5.5217400 | -2.2728500 | 2.6687400 |
| O29  | 5.5217400 | -2.2731600 | -2.6684700 |
| O30  | 5.8410700 | -2.6073900 | 1.8890700 |
| C31  | -7.1342600 | -2.3364100 | 0.4818700 |
| C32  | 7.1342700 | -2.3364700 | -0.4815900 |
| C33  | -7.8123600 | -3.4770100 | 0.9076600 |
| C34  | -9.1998400 | -3.4902300 | 0.9894600 |
| C35  | -9.9424400 | -2.3543600 | 0.6397000 |
| C36  | -9.2496200 | -1.2176800 | 0.2228900 |
| C37  | -7.8453900 | -1.1737600 | 0.1305100 |
| C38  | 7.8453900 | -1.1737800 | -0.1303600 |
| C39  | 9.2496200 | -1.2177000 | -0.2227400 |
| C40  | 9.9424500 | -2.3544300 | -0.6394200 |
C41  9.1998500  -3.4903400  -0.9890400
C42  7.8123600  -3.4771100  -0.9072400
C43  -1.2445200  4.8224300  -0.2615100
C44  -0.6942000  6.0856000  -0.1413600
C45   0.6942000  6.0856100   0.1406200
C46   1.2445100  4.8224700   0.2609200
S47  -0.0000020  3.6072400  -0.0002190
S48   3.1870500  2.8454200   0.0661100
C49   2.6052000  4.4302100   0.5582600
C50  -3.5979700  5.1285600   1.2354700
C51   4.8031100  4.3826800   1.3429500
C52   4.7596400  3.1238100   0.7819600
S53  -5.7834400  0.7714300  -0.3502600
C54  -5.7921200   2.1094100   0.7823500
C55   6.8759700   2.0051100   1.6310700
C56   7.6772200   0.8626000   1.3869600
C57   7.2203200   0.0635900   0.3611200
C58 -4.8031200   4.3825200  -1.3434800
C59  -3.5979700   5.1284100  -1.2360900
C60  -2.6052100   4.4301500  -0.5588000
S61  -3.1870500   2.8454200  -0.0664600
C62  -4.7596400   3.1237100  -0.7814300
C63  -7.6772300   0.8624300  -1.3870600
C64 -6.8759800   2.0049200  -1.6313000
C65  -5.7921300   2.1093200  -0.7826000
S66  -5.7834400   0.7714700   0.3501600
C67  -7.2203200   0.0635500  -0.3611300
C68  11.4512200  -2.3627100  -0.7163300
C69 -11.4512100  -2.3626400   0.7166200
C70 -3.4443900   6.5053400  -1.8253500
C71  3.4443900   6.5055500   1.8245700
H72   3.6621800  -2.6416200   3.1031900
H73   1.2096400  -2.6331000   3.3140400
H74   0.7446200  -2.3939900  -3.4480400
H75  -3.2019800  -2.3250900  -3.5724300
H76  -3.6621800  -2.6419800  -3.1028800
H77  -1.2096400  -2.6334900  -3.3137200
H78  -0.7446200  -2.3935800   3.4483200
H79  -3.2019700  -2.3246700   3.5727100
H80  -9.7093400  -4.3884700   1.3294000
H81  -9.8062600  -0.3175300  -0.0218800
H82   9.8062600  -0.3175200   0.0219200
H83   9.7093400  -4.3886200  -1.3288800
H84  -1.2768500   6.9938100  -0.2300500
H85  -1.2768500   6.9938400   0.2292000
H86   5.6904800   4.7735900   1.8303300
H87   7.0608600   2.7068400   2.4368700
H88   8.5440500   0.6004700   1.9836000
H89  -5.6904900   4.7733700  -1.8308900
H90  -8.5440600   0.6002400  -1.9836600
H91 -7.0608700 2.7065500 -2.4371800
H92 11.8663000 -1.3632600 -0.5542300
H93 11.8831300 -3.0292000 0.0412000
H94 11.7992200 -2.7176600 -1.6935100
H95 -11.8831200 -3.0292100 -0.0408300
H96 -11.7992100 -2.7174700 1.6938400
H97 -11.8663000 -1.3632000 0.5544100
H98 -4.1968100 6.6777100 -2.6014600
H99 -3.5711300 7.2918800 -1.0693100
H100 -2.4547000 6.6412500 -2.2745000
H101 2.4546800 6.6415200 2.2736900
H102 3.5711300 7.2920100 1.0684400
H103 4.1967900 6.6780200 2.6006700
H104 7.2379700 -4.3591700 -1.1720700
H105 -7.2379700 -4.3591700 1.1720700

Final geometry:

Total energy: −7544.84772028 Hartrees
C1 -2.8754100 -0.1459000 -2.4185000
C2 -1.4773400 -0.1128900 -2.4281000
C3 -0.7341900 -0.0306600 -1.2490700
C4 -1.4317400 -0.0009190 -0.0001740
C5 -2.8607500 -0.0008510 -0.0003510
C6 -3.5706500 -0.0803700 -1.2232800
C7 -0.7344900 0.0287800 1.2488900
C8 -1.4779100 0.1110600 2.4277400
C9 -2.8759800 0.1442100 2.4178000
C10 -3.5709200 0.0787600 1.2224100
C11 -5.0501900 -0.1201900 -1.2474300
C12 -5.0504600 0.1188600 1.2462100
C13 0.7344800 0.0285200 -1.2488900
C14 0.7341800 -0.0304000 1.2490800
C15 1.4317400 -0.0009200 0.0001770
C16 2.8607400 -0.0008530 0.0003540
C17 3.5706400 -0.0801200 1.2233000
C18 2.8754100 -0.1454000 2.4185300
C19 1.4779100 -0.1123800 2.4277700
C20 1.4779100 0.1105500 -2.4277700
C21 2.8759700 0.1437100 -2.4178300
C22 3.5709200 0.0785000 -1.2224200
C23 5.0504500 0.1186100 -1.2462300
C24  5.0501900  -0.1199400  1.2474600
N25  -5.7018600  -0.0006340  -0.0007020
N26  5.7018600  -0.0006390  0.0007050
O27  5.6947500  -0.2537200  2.2753800
O28  5.6952200  0.2526100  -2.2739700
O29  -5.6952300  0.2518000  2.2753200
C31  7.1450100  -0.0009150  0.0011800
C32  -7.1450100  -0.0009070  -0.0011700
C33  7.8400100  -1.1625100  -0.3883500
C34  9.2437300  -1.1357700  -0.3823900
C35  9.9604500  -0.0009390  -0.0007000
C36  9.2442500  1.1356500  0.3766100
C37  7.8403900  1.1615300  0.3873500
C38  -7.8403900  1.1614600  -0.3875900
C39  -9.2442500  1.1355800  -0.3768500
C40  -9.9604500  -0.0009300  0.0006940
C41  -9.2437300  -1.1356900  0.3826100
C42  -7.8400100  -1.1624300  0.3885800
C43  1.2247100  7.1553700  0.3419900
C44  0.6834800  8.4183500  0.1856500
C45  -0.6834800  8.4183100  -0.1872800
C46  -1.2247000  7.1553000  -0.3433900
S47  0.0000060  5.9400300  -0.0005890
S48  -3.1850700  5.1863100  -0.2682000
C49  -2.5633500  6.7643000  -0.7319500
C50  -3.5024100  7.4597600  -1.4844600
C51  -4.7002200  6.7168100  -1.6711100
C52  -4.7017800  5.4634900  -1.0962100
S53  -5.8346700  3.1473900  0.0022900
C54  -5.7305300  4.4467500  -1.1691900
C55  -6.7179000  4.3061200  -2.1233700
C56  -7.5318300  3.1619700  -1.9292000
C57  -7.1778400  2.3986800  -0.8381800
C58  4.7002200  6.7171300  1.6698000
C59  3.5024100  7.4600500  1.4830100
C60  2.5633600  6.7644400  0.7306300
S61  3.1850800  5.1863700  0.2671700
C62  4.7017900  5.4637000  1.0951300
C63  7.5318400  3.1623500  1.9285700
C64  6.7179100  4.3065400  2.1225100
C65  5.7305400  4.4469800  1.1683100
S66  5.8346700  3.1473900  -0.0029100
C67  7.1778400  2.3988500  0.8376900
C68  -11.4710000  -0.0108100  -0.0276300
C69  11.4710000  -0.0108200  0.0276700
C70  3.3014400  8.8310100  2.0719800
C71  -3.3014400  8.8306100  -2.0736900
H72  -3.4366800  -0.2197800  -3.3437800
H73  -0.9753500  -0.1628400  -3.3869500

S43
H74  -0.9761500  0.1609700  3.3867200
H75  -3.4374700  0.2174800  -3.3429800
H76   3.4366700  -0.2190800  3.3438300
H77   0.9753500  -0.1621300  3.3869900
H78   0.9761500  0.1602600  -3.3867500
H79  -3.4374700  0.2174800  -3.3429800
H80   9.7779900 -2.0373700  -0.6680200
H81   9.7788500  2.0398800   0.6529900
H82  -9.7788500  2.0397500  -0.6534200
H83  -9.7779900 -2.0372300   0.6684200
H84  1.2592400  9.3265100   0.3125200
H85  -1.2592400  9.3264400  -0.3143200
H86  -5.5492200  7.1054300  -2.2243200
H87  -6.8188500  4.9788000  -2.9679200
H88  -8.3274800  2.8705300  -2.6061600
H89  5.5492200  7.1058600   2.2229400
H90  8.3275000  2.8710500   2.6055800
H91  6.8188700  4.9793900   2.9669200
H92  -11.8803000  0.9894800   0.1475700
H93  -11.8454300 -0.3516300  -1.0019200
H94  -11.8814700 -0.6838200   0.7322900
H95  11.8453900 -0.3511700   1.0021400
H96  11.8814800 -0.6842100  -0.7319100
H97  11.8803200  0.9893800  -0.1480000
H98  3.9897900   8.9957000   2.9070300
H99  3.4872200  9.6251000   1.3362700
H100  2.2790900  8.9623100   2.4422800
H101 -2.2790800  8.9618500  -2.4440200
H102 -3.9897800  8.9951400  -2.9087800
H103 -3.4872200  9.6248300  -1.3381300
C104 -7.1761600  -2.3975400   0.8434600
S105 -5.8372800  -3.1504100  -0.0000470
C106 -7.5251800  -3.1554900   1.9396700
C107 -5.7278300  -4.4443600   1.1770100
C108 -6.7105100  -4.2990000   2.1352400
H109 -8.3174900  -2.8605900   2.6190500
C110 -4.6994700  -5.4615000   1.1036500
H111 -6.8074500  -4.9677000   2.9834200
S112 -3.1848600  -5.1858500   0.2713000
C113 -4.6964300  -6.7136400   1.6810500
C114 -2.5619100  -6.7628500   0.7366400
C115 -3.4989800  -7.4569000   1.4928400
H116 -5.5440900  -7.1011900   2.2370800
C117 -1.2240300  -7.1542100   0.3456500
C118 -3.2962900  -8.8266200   2.0841000
C119 -0.6831600  -8.4172200   0.1885800
S120 -0.0000000  -5.9389400   0.0005770
H121 -2.2724800  -8.9575700   2.4504900
H122 -3.9813000  -8.9891300   2.9232300
H123 -3.4854400  -9.6222600   1.3509200
C124  0.6831500   -8.4172600  -0.1869400
H125  -1.2587700   -9.3253100   0.3167400
C126  1.2240200   -7.1542800  -0.7353200
H127  -1.2587600  -9.3253700  -0.3149200
C128  2.5619000   -6.7630000  -0.3442600
C129  3.4989800   -7.4572000  -1.4913800
S130  3.1848600   -5.1859100  -0.2702900
C131  4.6964300   -6.7139800  -1.6797300
C132  3.2962800   -8.8270400  -2.0823700
C133  4.6994700   -5.4617200  -1.1025800
H134  5.5440900   -7.1016400  -2.2356800
H135  3.9813000  -9.39897100  -2.9205500
H136  3.4854300  -9.6225300  -1.3490300
H137  2.2724800  -8.9580600  -2.4487400
C138  5.7278300  -4.4446000  -1.1761400
C139  6.7105200  -4.2994400  -2.1343800
S140  5.8372600  -3.1504000   0.0006570
C141  7.5251900  -3.1558900  -1.9390300
H142  6.8074800  -4.9683100  -2.9824200
C143  7.1761500  -2.3977100  -2.6184700
H144  8.3175100  -2.8611400  -2.6184700

Final geometry:

![Chemical structure]

Total energy: $-9754.49276862$ Hartrees

C1  0.95871  -2.71421  -2.56024
C2  0.51661  -1.38751  -2.56859
C3  0.24216  -0.69402  -1.3882
C4  0.4409  -1.36277  -0.1387
C5  0.87715  -2.72411  -0.13926
C6  1.1322  -3.38817  -1.36398
C7  0.21252  -0.70384  1.11108
C8  0.40472  -1.42547  2.29081
C9  0.81396  -2.76296  2.28128
C10  1.05364  -3.41505  1.08438
C11  1.58437  -4.79821  -1.39089
C12  1.46155  -4.8392  1.10759
C13  -0.24255  0.69396  -1.3882
C14  -0.21281  0.70382  1.11108
C15  -0.44122  1.36274  -0.13871
|   |   |   |   |
|---|---|---|---|
|C16| -0.87741 | 2.7241 | -0.13927 |
|C17| -1.0538 | 3.41507 | 1.08437 |
|C18| -0.81411 | 2.76299 | 2.28127 |
|C19| -0.40493 | 1.42548 | 2.29081 |
|C20| -0.51706 | 1.38743 | -2.56858 |
|C21| -0.9591 | 2.71415 | -2.56024 |
|C22| -1.1325 | 3.38814 | -1.36399 |
|C23| -1.58457 | 4.79822 | -1.39089 |
|C24| -1.46159 | 4.83925 | 1.10758 |
|N25| 1.70772 | -5.44122 | -0.14375 |
|N26| -1.70777 | 5.44126 | -0.14377 |
|O27| -1.57246 | 5.48079 | 2.13996 |
|O28| -1.84329 | 5.39108 | -2.42724 |
|O29| 1.57249 | -5.48071 | 2.13999 |
|O30| 1.84306 | -5.39107 | -2.42724 |
|C31| -2.03734 | 6.84718 | -0.14897 |
|C32| 2.03742 | -6.8471 | -0.14899 |
|C33| -1.00602 | 7.7706 | -0.39203 |
|C34| -1.29934 | 9.13746 | -0.38794 |
|C35| -2.59432 | 9.60371 | -0.13747 |
|C36| -3.59832 | 8.66518 | 0.09794 |
|C37| -3.35116 | 7.28051 | 0.09949 |
|C38| 1.06619 | -7.77062 | -0.39214 |
|C39| 1.29968 | -9.13744 | -0.38829 |
|C40| 2.59475 | -9.60357 | -0.13795 |
|C41| 3.59862 | -8.66496 | 0.09763 |
|C42| 3.35128 | -7.28031 | 0.0994 |
|C43| -9.56894 | -2.65015 | -0.16738 |
|C44| -9.14967 | -3.03108 | -1.4309 |
|C45| -7.99508 | -3.84264 | -1.43564 |
|C46| -7.48542 | -4.10944 | -0.17662 |
|S47| -8.48308 | -3.32469 | 1.04094 |
|S48| -5.06813 | -5.05809 | -1.1052 |
|C49| -6.2809 | -4.83962 | 0.15355 |
|C50| -5.86642 | -5.43159 | 1.34004 |
|C51| -4.60028 | -6.06716 | 1.21144 |
|C52| -4.03002 | -5.98035 | -0.03904 |
|S53| -1.45717 | -6.82406 | 0.62588 |
|C54| -2.75963 | -6.49492 | -0.50441 |
|C55| -2.35039 | -6.75894 | -1.79412 |
|C56| -1.00953 | -7.22358 | -1.88072 |
|C57| -0.37949 | -7.31839 | -0.66523 |
|C58| -12.32501 | -0.51891 | 1.22699 |
|C59| -11.06539 | -1.17284 | 1.33167 |
|C60| -10.74404 | -1.88072 | 0.17949 |
|S61| -12.03979 | -1.75496 | -1.00756 |
|C62| -5.42538 | 6.55805 | 1.37624 |
|C63| -6.43032 | 5.55739 | 1.39935 |
|S64| -4.86363 | 4.95543 | -0.55699 |
|C65| -4.47902 | 6.3794 | 0.39232 |
| C66 | 2.89148 | -11.08473 | -0.11626 |
| C67 | -2.89088 | 11.08491 | -0.11536 |
| C68 | -10.20018 | -1.05286 | 2.55991 |
| C69 | -6.64122 | -5.44927 | 2.63239 |
| H70 | 1.16789 | -3.23723 | -3.48728 |
| H71 | 0.39292 | -0.90131 | -3.52885 |
| H72 | 0.94793 | -3.31063 | 3.20801 |
| H73 | -0.948 | 3.31068 | 3.208 |
| H74 | -0.23048 | 0.9568 | 3.25192 |
| H75 | -0.39344 | 0.9012 | -3.52884 |
| H77 | -1.16832 | 3.23715 | -3.48728 |
| H78 | -0.49585 | 9.84259 | -0.58281 |
| H79 | -4.61693 | 9.00367 | 0.26397 |
| H80 | 0.49628 | -9.84265 | -0.58319 |
| H81 | 4.61727 | -9.00334 | 0.26362 |
| H82 | -9.66794 | -2.72943 | -2.33492 |
| H83 | -7.54371 | -4.22903 | -2.34315 |
| H84 | -4.1323 | -6.60533 | 2.02995 |
| H85 | -2.99969 | -6.63404 | -2.65442 |
| H86 | -0.50912 | -7.46306 | -2.81222 |
| H87 | -12.7242 | 0.1038 | 2.02177 |
| H88 | -5.37169 | 7.37131 | 2.09184 |
| H89 | -7.22762 | 5.52323 | 2.13422 |
| H90 | 2.54746 | -11.54272 | 0.82023 |
| H91 | 2.38488 | -11.606 | -0.93604 |
| H92 | 3.96499 | -11.27884 | -0.20335 |
| H93 | -2.54828 | 11.54226 | 0.82197 |
| H94 | -2.3829 | 11.6066 | -0.93401 |
| H95 | -3.96423 | 11.27922 | -0.20399 |
| H96 | -10.58985 | 0.27564 | 3.22445 |
| H97 | -10.16968 | -1.98803 | 3.13314 |
| H98 | -9.16748 | -0.78914 | 2.30662 |
| H99 | -7.69823 | -5.68883 | 2.4736 |
| H100 | -6.22605 | -6.19808 | 3.31406 |
| H101 | -6.60138 | -4.48086 | 3.14771 |
| C102 | 4.47904 | -6.37912 | 0.39237 |
| S103 | 4.8634 | -4.95483 | -0.55655 |
| C104 | 5.4255 | -6.55791 | 1.37619 |
| C105 | 6.4303 | -5.55712 | 1.3995 |
| H106 | 5.37196 | -7.37136 | 2.09158 |
| H107 | 7.22765 | -5.52308 | 2.13432 |
| S108 | 12.03952 | 1.75412 | -1.00799 |
| C109 | 12.32566 | 0.5195 | 1.22724 |
| C110 | 10.74416 | 1.88044 | 0.17943 |
| C111 | 11.06599 | 1.17332 | 1.33193 |
| H112 | 12.72519 | -0.10265 | 2.02228 |
| C113 | 9.56885 | 2.6495 | -0.16754 |
| C114 | 10.20118 | 1.05398 | 2.56052 |
| C115 | 9.1488 | 3.02909 | -1.4312 |
| Atom | X  | Y  | Z  | Element |
|------|----|----|----|---------|
| S116 | 8.48375 | 3.32533 | 1.04074 |
| H117 | 9.16831 | 0.79055 | 2.30769 |
| H118 | 10.59084 | 0.27683 | 3.22515 |
| H119 | 10.17122 | 1.98934 | 3.13348 |
| C120 | 7.99418 | 3.84061 | -1.43609 |
| H121 | 9.6665 | 2.72647 | -2.33522 |
| C122 | 7.48528 | 4.10873 | -0.17703 |
| H123 | 7.54223 | 4.226 | -2.34374 |
| C124 | 6.28096 | 4.83926 | 0.1531 |
| C125 | 5.8669 | 5.4319 | 1.3394 |
| S126 | 5.06784 | 5.05724 | -1.10541 |
| C127 | 5.00081 | 6.06757 | 1.21084 |
| C128 | 6.64206 | 5.45013 | 2.63153 |
| C129 | 4.03016 | 5.98018 | -0.03942 |
| H130 | 4.13313 | 6.6062 | 2.02922 |
| H131 | 6.22671 | 6.19884 | 3.31321 |
| H132 | 6.60284 | 4.48178 | 3.147 |
| C133 | 7.99891 | 5.69019 | 2.47241 |
| C124 | 2.75969 | 6.49463 | -0.50469 |
| C135 | 2.35011 | 6.75795 | -1.79443 |
| S136 | 1.45757 | 6.82449 | 0.62578 |
| C137 | 1.00926 | 7.22264 | -1.88093 |
| H138 | 2.99917 | 6.63254 | -2.65484 |
| C139 | 0.37957 | 7.31819 | -0.66532 |
| H140 | 0.50861 | 7.46162 | -2.81243 |
| C141 | -14.2592 | -0.18225 | -0.4033 |
| C142 | -14.77335 | -0.09534 | -1.68033 |
| S143 | -15.41243 | 0.4595 | 0.75702 |
| C144 | -16.07116 | 0.4863 | -1.73296 |
| H145 | -14.22464 | -0.42141 | -2.55759 |
| C146 | -16.54515 | 0.8429 | -0.50036 |
| H147 | -16.62456 | 0.6399 | -2.65295 |
| H148 | -17.49017 | 1.30623 | -0.25098 |
| C149 | -7.09219 | 3.43258 | 0.14921 |
| C150 | -6.74985 | 2.25473 | -0.47981 |
| S151 | -8.77987 | 3.38925 | 0.63507 |
| C152 | -7.8214 | 1.31988 | -0.56121 |
| H153 | -5.74932 | 2.05814 | -0.85046 |
| C154 | -8.97783 | 1.78498 | 0.00314 |
| H155 | -7.73402 | 0.33675 | -1.01094 |
| H156 | -9.93316 | 1.28411 | 0.0865 |
| C157 | 7.09187 | -3.43193 | 0.14986 |
| C158 | 6.74945 | -2.25402 | -0.479 |
| S159 | 8.77952 | -3.38849 | 0.63583 |
| C160 | 7.82091 | -1.31904 | -0.5602 |
| H161 | 5.74892 | -2.05748 | -0.8497 |
| C162 | 8.97735 | -1.78411 | 0.00416 |
| H163 | 7.73347 | -0.33586 | -1.00981 |
| H164 | 9.93261 | -1.28315 | 0.08767 |
| C165 | 6.27316 | -4.59751 | 0.42265 |
C166 -6.27337 4.59802 0.42223
C167 -12.98258 -0.70718 0.03077
C168 14.25936 0.18208 -0.40348
C169 14.77352 0.09539 -1.68053
S170 15.41245 -0.46018 0.7567
C171 16.07123 -0.48646 -1.73328
H172 14.22492 0.42181 -2.55772
C173 16.54514 -0.84345 -0.50076
H174 16.62463 -0.6399 -2.6533
H175 17.49007 -1.307 -0.25146
C176 12.98282 0.70714 0.03068

Final geometry:

Total energy: -5813.16854119 Hartrees

| Atom |  X   |  Y   |  Z   |
|------|------|------|------|
| C1   | 0.21155 | 5.03336 | 2.21321 |
| C2   | 1.42403 | 4.3359 | 2.22778 |
| C3   | 2.0176 | 3.86163 | 1.05631 |
| C4   | 1.35849 | 4.10387 | -0.1908 |
| C5   | 0.11958 | 4.81776 | -0.19664 |
| C6   | -0.44424 | 5.27602 | 1.01895 |
| C7   | 1.90607 | 3.6475 | -1.43197 |
| C8   | 1.20926 | 3.9224 | -2.61034 |
| C9   | -0.00184 | 4.62223 | -2.60752 |
| C10  | -0.55118 | 5.06888 | -1.41836 |
| C11  | -1.72666 | 6.0215 | 1.03876 |
| C12  | -1.841 | 5.79954 | -1.44974 |
| C13  | 3.28697 | 3.11894 | 1.06327 |
| C14  | 3.17326 | 2.90128 | -1.42458 |
| C15  | 3.82789 | 2.65121 | -0.1766 |
| C16  | 5.0511 | 1.91085 | -0.1679 |
| C17  | 5.60316 | 1.43389 | -1.38161 |
| C18  | 4.95879 | 1.69592 | -2.57805 |
| C19  | 3.7619 | 2.41939 | -2.59539 |
| C20  | 3.98478 | 2.84527 | 2.2414 |
| C21  | 5.18015 | 2.11902 | 2.24136 |
| C22  | 5.71477 | 1.64724 | 1.05511 |
| C23  | 6.96356 | 0.84936 | 1.09407 |
| C24  | 6.85936 | 0.64647 | -1.39696 |
| N25  | -2.35424 | 6.22396 | -0.20857 |
| N26  | 7.44781 | 0.37892 | -0.14211 |
| O27  | 7.36814 | 0.23635 | -2.42707 |
| O28  | 7.54641 | 0.58686 | 2.13497 |
|   |   |   |   |
|---|---|---|---|
| O29 | -2.44515 | 6.02502 | -2.48681 |
| O30 | -2.22478 | 6.44743 | 2.06756 |
| C31 | 8.6396   | -0.43938 | -0.13325 |
| C32 | -3.59053 | 6.97454 | -0.21385 |
| C33 | 9.88077  | 0.18714  | -0.05074 |
| C34 | 11.05342 | -0.59958 | -0.09127 |
| C35 | 11.00642 | -1.95356 | -0.22507 |
| C36 | 9.75415  | -2.56705 | -0.29641 |
| C37 | 8.5529   | -1.83822 | -0.25025 |
| C38 | -4.8202  | 6.36513  | 0.09139  |
| C39 | -5.96416 | 7.18511  | 0.11192  |
| C40 | -5.91534 | 8.55409  | -0.15391 |
| C41 | -4.6737  | 9.12323  | -0.46657 |
| C42 | -3.52652 | 8.33858  | -0.49216 |
| C43 | -0.08954 | -5.10065 | 0.33072  |
| C44 | -0.40973 | -6.06761 | -0.60532 |
| C45 | -1.79094 | -6.34613 | -0.69512 |
| C46 | -2.57609 | -5.59999 | 0.16703  |
| S47 | -1.55614 | -4.51321 | 1.10046  |
| S48 | -4.95993 | -6.31628 | -1.01777 |
| C49 | -4.01626 | -5.62925 | 0.30212  |
| C50 | -4.85019 | -5.19765 | 1.32704  |
| C51 | -6.22224 | -5.45155 | 1.04622  |
| S52 | -4.31141 | 3.6417   | -0.55495 |
| S53 | -5.76734 | 2.99678  | 1.47194  |
| C54 | -5.74329 | 4.41494  | 1.4386   |
| S55 | -4.98482 | 4.93834  | 0.41593  |
| C56 | 3.07108  | -3.57779 | 1.65875  |
| C57 | 1.71112  | -3.97014 | 1.79506  |
| C58 | 1.21604  | -4.55588 | 0.63765  |
| S59 | 2.44593  | -4.58372 | -0.62241 |
| C60 | 3.6336   | -3.8418  | 0.42892  |
| C61 | 6.94679  | -3.52268 | -1.2948  |
| C62 | 5.65099  | -4.07457 | -1.1208  |
| C63 | 4.97143  | -3.55382 | -0.03913 |
| S64 | 5.9607   | -2.35792 | 0.77846  |
| C65 | 7.27767  | -2.56862 | -0.36002 |
| C66 | -7.16559 | 9.40098  | -0.10837 |
| C67 | 12.27721 | -2.76794 | -0.29075 |
| C68 | 0.94795  | -3.77677 | 3.08035  |
| C69 | -4.40575 | -4.5542  | 2.61568  |
| H70 | -0.23502 | 5.39283  | 3.13415  |
| H71 | 1.89801  | 4.16683  | 3.18726  |
| H72 | 1.59838  | 3.58987  | -3.5652  |
| H73 | -0.53109 | 4.82287  | -3.53296 |
| H74 | 5.39752  | 1.32374  | -3.49768 |
| H75 | 3.29151  | 2.5948   | -3.55544 |
| H76 | 3.60335  | 3.19085  | 3.19476  |
| H77 | 5.7026   | 1.90716  | 3.16819  |
| H78 | 12.0136  | -0.05443 | -0.02079 |
|   |     |     |     |
|---|-----|-----|-----|
| H79 | 9.69342 | -3.64926 | -0.37128 |
| H80 | -6.92213 | 6.71874 | 0.32363 |
| H81 | -4.60403 | 10.18466 | -0.69135 |
| H82 | 0.3429 | -6.58438 | -1.19108 |
| H83 | -2.20337 | -7.10041 | -1.35668 |
| H84 | -7.0128 | -5.21296 | 1.75115 |
| H85 | -6.28506 | 2.42199 | 2.2326 |
| H86 | -6.24043 | 5.04186 | 2.17084 |
| H87 | 3.63232 | -3.12977 | 2.47304 |
| H88 | 7.61429 | -3.79672 | -2.1045 |
| H89 | 5.23052 | -4.83559 | -1.76987 |
| H90 | -8.06577 | 8.783 | -0.03602 |
| H91 | -7.15561 | 10.07583 | 0.75726 |
| H92 | -7.25694 | 10.02679 | -1.00375 |
| H93 | 12.80193 | -2.60718 | -1.24134 |
| H94 | 12.97116 | -2.49086 | 0.51127 |
| H95 | 12.07162 | -3.83918 | -0.20335 |
| H96 | 1.64092 | -3.63127 | 3.91512 |
| H97 | 0.29539 | -2.89495 | 3.04075 |
| H98 | 0.31486 | -4.63877 | 3.31385 |
| H99 | -4.09834 | -3.51132 | 2.46583 |
| H100 | -5.22573 | -4.55195 | 3.34057 |
| H101 | -3.55968 | -5.08281 | 3.06759 |
| H102 | -2.56255 | 8.78133 | -0.72349 |
| H103 | 9.91891 | 1.26833 | 0.03849 |
| C104 | -7.72916 | -6.46649 | -0.74549 |
| C105 | -7.96477 | -7.33151 | -1.79389 |
| S106 | -9.24963 | -5.83759 | -0.12837 |
| C107 | -9.3456 | -7.49723 | -2.09577 |
| H108 | -7.16852 | -7.84793 | -2.31954 |
| C109 | -10.16093 | -6.76199 | -1.27984 |
| H110 | -9.71559 | -8.1437 | -2.88408 |
| H111 | -11.24095 | -6.70331 | -1.28355 |
| C112 | -4.82908 | 1.00199 | 0.18352 |
| C113 | -3.79324 | 0.388 | -0.48724 |
| S114 | -6.0057 | -0.19485 | 0.70245 |
| C115 | -3.93059 | -1.02678 | -0.57539 |
| H116 | -2.94695 | 0.93729 | -0.88609 |
| C117 | -5.06873 | -1.49043 | 0.02613 |
| H118 | -3.20742 | -1.67441 | -1.05885 |
| H119 | -5.41881 | -2.51124 | 0.10583 |
| C120 | -6.46746 | -6.06139 | -0.16475 |
| C121 | -5.03165 | 2.41035 | 0.46483 |
Final geometry:

![Chemical structure](image)

Total energy: $-1104.81669881$ Hartrees

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C1   | 0     | 3.21057 | -0.05036 |
| C2   | -1.26892 | 2.7657 | 0.19851 |
| C3   | -1.35485 | 1.34567 | 0.26702 |
| S4   | 1.11645 | 1.89317 | -0.22313 |
| H5   | 0.3497 | 4.22987 | -0.14378 |
| H6   | -2.11707 | 3.42706 | 0.33872 |
| H7   | -2.27318 | 0.80799 | 0.4783 |
| C8   | 0.14867 | -0.71017 | 0.06763 |
| C9   | 1.35485 | -1.34567 | 0.26702 |
| S10  | -1.11645 | -1.89317 | -0.22313 |
| C11  | 1.26892 | -2.7657 | 0.19851 |
| H12  | 2.27318 | -0.80799 | 0.4783 |
| C13  | 0     | -3.21057 | -0.05036 |
| H14  | 2.11707 | -3.42706 | 0.33872 |
| H15  | -0.3497 | -4.22987 | -0.14378 |
| C16  | -0.14867 | 0.71017 | 0.06763 |
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