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Supporting Information

The smallest oligothiophene diradicals by asymmetric substitution of quinoidal cores

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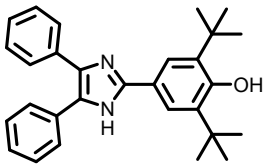
1. General information

All chemicals and reagents were purchased from Alfa, Acros and Adamas without further purifications. Anhydrous tetrahydrofuran (THF) was distilled over sodium under a nitrogen atmosphere. Column chromatography was performed on Haiyang silica gel (200-300 mesh). All reactions were monitored by thin layer chromatography (TLC) using commercial Huanghai glass plates (HSGF 254, 2.5 x 8 cm) visualized under UV radiation at 254 and 365 nm. The acid sensitive compounds were purified with trimethylamine pretreated silica gel and all organic extracts were dried by anhydrous Na2SO4. UV/Vis/NIR absorption spectra were performed using a Shimadzu UV-2600 UV-VIS spectrophotometer. MALDI-TOF massspectra (MS) were measured on a SHIMADZU iD plus Performance using anthracene-1, 8, 9-triol as matrix. High resolution mass spectra (HRMS) were recorded on a Waters-Q-TOF-Premier (ESI). NMR spectra were measured by a Bruker AV III HD 400 MHz. ESR spectroscopy measurement was conducted by a Bruker EMX plus X-band spectrometer with 9.8 GHz microwave frequency. Elemental analysis measurements were performed on a Leeman Labs Euro EA 3000 elemental analyzer. Single Crystal X-Ray Diffraction were measured by a Gemini X-ray Single Crystal Diffractometer. Cyclic voltammograms were measured on a Shanghai Chenhua CHI 660E electrochemical workstation. The Raman spectra were recorded by Bruker Senterra Raman microscope by averaging spectra during 50 min with a resolution of 3–5 cm^{-1}. The spectra were collected using a 1 × 1 CCD camera of the mentioned microscope. Variable temperature electronic UV-Vis absorption spectra were recorded in a Varian Cary 5000 UV-Vis-NIR spectrophotometer.

2. Preparation of materials

2.1 Synthesis of PTI-0

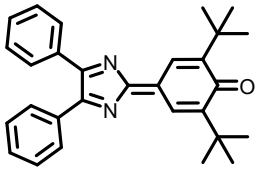
Synthesis of 2



2

3,5-di-tert-butyl-4-hydroxybenzaldehyde[**1**] (300 mg, 1.28 mmol, 1.0 eq), benzil (269 mg, 1.28 mmol, 1.0 eq) and ammonium acetate (888 mg, 11.52 mmol, 9.0 eq) were charged in a 100 mL of two neck flask with 20 mL acetic acid under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. Hot dichloromethane was added to the residue until it just dissolved and then recrystallized in -20 ℃ to give [**2**] as a white solid (488 mg, 90%). ^{1}H NMR (400 MHz, DMSO-d6): δ = 12.50 (1 H, s), 7.81 (2 H, s), 7.49 (2 H, d, J_{HH} = 8 Hz), 7.35 (2 H, m), 7.33 (4 H, m), 7.16 (1 H, s), 1.45 (CH_3, 18 H, s). ^{13}C NMR (100 MHz, DMSO-d6): δ = 150.40, 146.78, 139.25, 128.60, 128.49, 128.41, 127.68, 127.10, 122.24, 122.20, 34.75, 30.44. MALDI-TOF m/z: [M]+ calcd. for $C_{29}H_{32}N_2O$ 424.25, found 424.05.

Synthesis of PTI-0



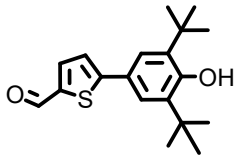
PTI-0

Compound **2** (50 mg, 0.12 mmol, 1.0 eq) and lead (IV) oxide (144 mg, 0.6 mmol, 5.0 eq) were charged in a 50 mL two neck flask with 10 mL of dichloromethane. The

mixture was stirred at room temperature for 30 min. After stirring the reaction mixture at room temperature for 30 minutes the excess lead oxide was filtered off and the solvent was removed under reduced pressure. The product was purified by column chromatography (neutral alumina, hexane/DCM, V/V = 4: 1, as eluent) to give **PTI-0** as a brown solid (41 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.36 (2 H, s), 7.77 (4 H, d, J_{HH} = 8 Hz), 7.53 (2 H, m), 7.44 (4 H, m), 1.41 (CH_3, 18 H, s). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 187.34, 168.44, 165.39, 153.24, 133.77, 132.79, 131.33, 130.01, 129.21, 128.67, 36.38, 29.97. MALDI-TOF m/z: [M]+ calcd. for $C_{29}H_{30}N_2O$ 422.24, found 422.10.

2.2 Synthesis of PTI-1

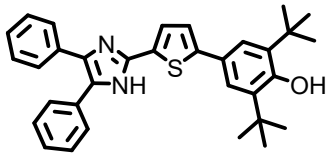
Synthesis of 4



4

5-bromothiophene-2-carbaldehyde[**3**] (191 mg, 1 mmol, 1.0 eq), 2,6-bis(1,1-dimethylethyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenol (332 mg, 1 mmol, 1.0 eq), tetrakis(triphenylphosphine)palladium(0) (58 mg, 0.05 eq) and sodium carbonate (848 mg, 8 mmol, 8.0 eq) were charged in a 100 mL two neck flask with 4 mL of water and 10 mL of tetrahydrofuran under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The product was purified by column chromatography (SiO_2, hexane/DCM, V/V = 5: 1, as eluent) to give [**4**] as a yellow solid (268 mg, 85%).[1] MALDI-TOF m/z: [M]+ calcd. for $C_{19}H_{24}O_2S$ 316.15, found 316.01.

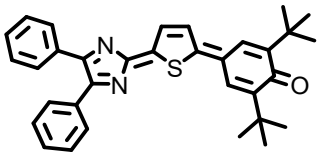
Synthesis of 5



5

Compound **4** (250 mg, 0.79 mmol, 1.0 eq), benzil (166 mg, 0.79 mmol, 1.0 eq) and ammonium acetate (548 mg, 7.11 mmol, 9.0 eq) were charged in a 100 mL two neck flask with 10 mL of acetic acid under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. Hot dichloromethane was added to the residue until it just dissolved and then recrystallized in -20 ℃ to give [**5**] as a white solid (364 mg, 91%). ^{1}H NMR (400 MHz, DMSO-d6): δ = 12.77 (1 H, s), 7.64 (1 H, d, J_{HH} = 4 Hz), 7.51 (4 H, m), 7.44 (2 H, m), 7.40 (4 H, m), 7.31 (2 H, m), 7.23 (2 H, m), 1.44 (CH_3, 18 H, s). ^{13}C NMR (100 MHz, DMSO-d6): δ = 154.19, 144.61, 141.56, 139.91, 136.87, 134.83, 131.58, 130.85, 128.72, 128.24, 127.09, 125.26, 122.72, 121.96. HRMS (ESI$^+$): calcd. for $C_{33}H_{34}N_2OS$ 506.2392, found $[M+H]^+$ 507.2478.

Synthesis of PTI-1



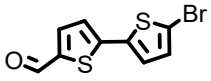
PTI-1

Compound **5** (50 mg, 0.10 mmol, 1.0 eq) and lead (IV) oxide (120 mg, 0.5 mmol, 5.0 eq) were charged in a 50 mL two neck flask with 10 mL of dichloromethane. The mixture was stirred at room temperature for 30 min. After stirring the reaction mixture at room temperature for 30 minutes the excess lead oxide was filtered off and the solvent was removed under reduced pressure. The product was purified by column chromatography (neutral alumina, hexane/DCM, V/V = 2: 1, as eluent) to give **PTI-1** as a blue solid (38 mg, 76%). ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.19 (2 H, d, J_{HH} =

8 Hz), 7.80 (4 H, m), 7.68 (4 H, d, J_{HH} = 8 Hz), 7.55 (4 H, d, J_{HH} = 8 Hz), 7.40 (1 H, s), 7.12 (1 H, s), 1.46 (CH_3, 18 H, s). ^{13}C NMR (100 MHz, DMSO-d6): δ =153.89, 145.24, 140.75, 139.60, 137.38, 131.20, 129.21, 128.45, 126.94, 126.67, 125.77, 123.04, 34.67, 30.34. HRMS (ESI^+): calcd. for C33H32N2OS 504.2235, found $[M+H]^+$ 505.2316.

2.3 Synthesis of PTI-2

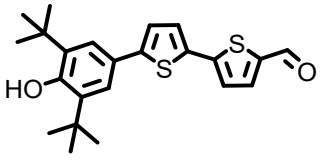
Synthesis of 7



7

5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophene-2-carbaldehyde[**6**] (2.00 g, 8.40 mmol, 1.0 eq), 2,5-dibromothiophene (2.03 g, 8.40 mmol, 1.0 eq), tetrakis(triphenylphosphine)palladium(0) (485 mg, 0.05 eq) and sodium carbonate (7.12 g, 67.20 mmol, 8.0 eq) were charged in a 250 mL two neck flask with 35 mL of water and 70 mL of tetrahydrofuran under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 250 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 100 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The product was purified by column chromatography (SiO_2, hexane/DCM, V/V = 3: 1, as eluent) to give [**7**] as a yellow solid (1324 mg, 58%).[2] MALDI-TOF m/z: [M]+ calcd. for $C_9H_5BrOS_2$ 271.90, found 271.75.

Synthesis of 8

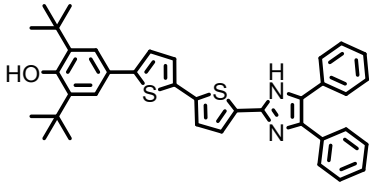


8

Compound **7** (500 mg, 1.84 mmol, 1.0 eq), 2,6-bis(1,1-dimethylethyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenol (612 mg, 1.84 mmol, 1.0 eq), tetrakis(triphenylphosphine)palladium(0) (106 mg, 0.05 eq) and sodium carbonate

(1.56 g, 14.72 mmol, 8.0 eq) were charged in a 100 mL of two neck flask with 8 mL of water and 20 mL of tetrahydrofuran under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The product was purified by column chromatography (SiO_2, hexane/DCM, V/V = 1: 1, as eluent) to give [**8**] as a yellow solid (542 mg, 74%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 9.84 (1 H, s), 7.69 (1 H, d, J_{HH} = 4 Hz), 7.44 (2 H, s), 7.35 (1 H, d, J_{HH} = 4 Hz), 7.27 (1 H, d, J_{HH} = 4 Hz), 7.18 (1 H, d, J_{HH} = 4 Hz), 5.42 (1 H, s), 1.49 (CH_3, 18 H, s). ^{13}C NMR (100 MHz, CD_2Cl_2): δ = 182.91, 155.01, 148.30, 147.75, 141.83, 138.12, 137.31, 134.23, 127.72, 125.51, 124.27, 123.52, 123.41, 34.90, 30.49. MALDI-TOF m/z: [M]+ calcd. for $C_{23}H_{26}O_2S_2$ 398.14, found 398.13.

Synthesis of 9

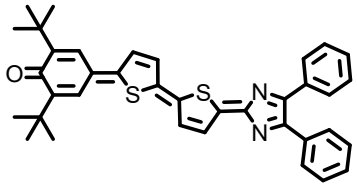


9

Compound **8** (300 mg, 0.75 mmol, 1.0 eq), benzil (158 mg, 0.75 mmol, 1.0 eq) and ammonium acetate (520 mg, 6.75 mmol, 9.0 eq) were charged in a 100 mL of two neck flask with 15 mL of acetic acid under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. Hot dichloromethane was added to the residue until it just dissolved and then recrystallized in -20 ℃ to give [**9**] as a yellow solid (273 mg, 62%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 9.55 (1 H, s), 7.54 (4 H, m), 7.43 (2 H, s), 7.35 (4 H, m), 7.32 (1 H, s), 7.31 (2 H, m), 7.20 (1 H, d, J_{HH} = 4 Hz), 7.18 (1 H, d, J_{HH} = 4 Hz), 7.14 (1 H, d, J_{HH} = 4 Hz), 5.37 (1 H, s), 1.49 (CH_3, 18 H, s). ^{13}C NMR (100

MHz, CD_2Cl_2): δ = 154.62, 145.80, 141.75, 138.73, 137.22, 135.21, 132.05, 129.10, 128.35, 125.92, 125.58, 124.80, 124.18, 123.37, 123.10, 34.89, 30.51. HRMS (ESI^+): calcd. for $C_{37}H_{36}N_2OS_2$ 588.2269, found $[M+H]^+$ 589.2347.

Synthesis of PTI-2

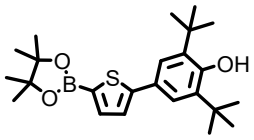


PTI-2

[**9**] (50 mg, 0.085 mmol, 1.0 eq) and lead (IV) oxide (102 mg, 0.425 mmol, 5.0 eq) were charged in a 50 mL of two neck flask with 10 mL dichloromethane. The mixture was stirred at room temperature for 30 min. After stirring the reaction mixture at room temperature for 30 minutes the excess lead oxide was filtered off and the solvent was removed under reduced pressure. The product was purified by column chromatography (neutral alumina, hexane/DCM, V/V = 2: 1, as eluent) to give **PTI-2** as a blue solid (38 mg, 76%). HRMS (ESI^+): calcd. for $C_{37}H_{36}N_2OS_2$ 586.2113, found $[M+H]^+$ 589.2343(HRMS used methanol as solvent, so the sample may be reduced to [**9**] by methanol). Maldi-Tof mass spectrum found $[M]^+$ 586.11.

2.4 Synthesis of PTI-3

Synthesis of 11

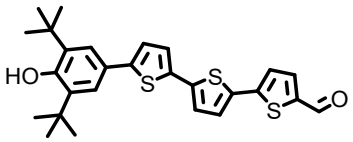


11

2,2'-(2,5-thiophenediyl)bis[4,4,5,5-tetramethyl-1,3,2-dioxaborolane][**10**] (6.43 g, 19.28 mmol, 1.1 eq), 4-bromo-2,6-bis(1,1-dimethylethyl)phenol (5.00 g, 17.53 mmol, 1.0 eq), tetrakis(triphenylphosphine)palladium(0) (1.01 g, 0.05 eq) and potassium acetate (4.65 mg, 47.33 mmol, 2.7 eq) were charged in a 250 mL two neck flask with 120 mL of 1,4-dioxane under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 250 mL of water was added, and

then the mixture was extracted with dichloromethane (3 x 100 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The product cannot be purified and was directly used for the next step.

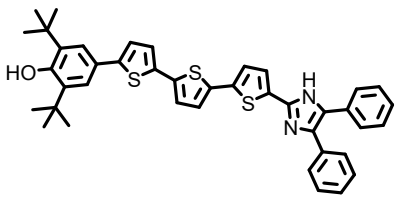
Synthesis of 12



12

Compound **7** (500 mg, 1.84 mmol, 1.0 eq), [**11**] (762 mg, 1.84 mmol, 1.0 eq), tetrakis(triphenylphosphine)palladium(0) (106 mg, 0.05 eq) and sodium carbonate (1.56 g, 14.72 mmol, 8.0 eq) were charged in a 100 mL of two neck flask with 8 mL of water and 20 mL of tetrahydrofuran under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The product was purified by column chromatography (SiO_2, hexane/DCM, V/V = 1: 2, as eluent) to give [**12**] as an orange solid (542 mg, 74%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 9.85 (1 H, s), 7.69 (1 H, d, J_{HH} = 4 Hz), 7.43 (2 H, s), 7.31 (4 H, d, J_{HH} = 4 Hz), 7.27 (1 H, d, J_{HH} = 4 Hz), 7.20 (1 H, d, J_{HH} = 4 Hz), 7.15 (2 H, m), 5.39 (1 H, s), 1.49 (CH_3, 18 H, s). ^{13}C NMR (100 MHz, CD_2Cl_2): δ = 182.92, 154.74, 147.04, 146.38, 142.18, 140.00, 138.04, 137.25, 134.70, 134.56, 127.61, 125.94, 125.77, 124.65, 123.38, 123.16, 34.89, 30.50. MALDI-TOF m/z: [M]+ calcd. for $C_{27}H_{28}O_2S_3$ 480.13, found 480.09.

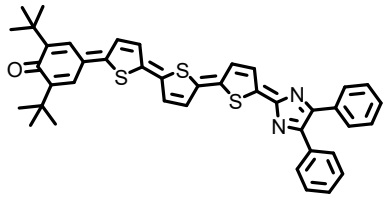
Synthesis of 13



13

Compound **12** (300 mg, 0.63 mmol, 1.0 eq), benzil (133 mg, 0.63 mmol, 1.0 eq) and ammonium acetate (437 mg, 5.67 mmol, 9.0 eq) were charged in a 100 mL of two neck flask with 15 mL of acetic acid under nitrogen. The mixture was shielded from light and heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. Hot dichloromethane was added to the residue until it just dissolved and then recrystallized in -20 ℃ to give [**9**] as a yellow solid (304 mg, 72%). ^{1}H NMR (400 MHz, DMSO-d6): δ = 12.90 (1 H, s), 7.93 (1 H, d, J_{HH} = 4 Hz), 7.64 (1 H, d, J_{HH} = 4 Hz), 7.52 (4 H, m), 7.37 (4 H, m), 7.33 (2 H, m), 7.27 (2 H, m), 6.89 (1 H, s), 6.71 (1 H, s), 5.76 (1 H, s), 5.33 (1 H, m), 1.44 (CH_3, 18 H, s). (Due to poor solubility, no NMR carbon spectrum) HRMS (ESI$^+$): calcd. for $C_{41}H_{38}N_2OS_3$ 670.2146, found [M+H]$^+$ 671.2226.

Synthesis of PTI-3

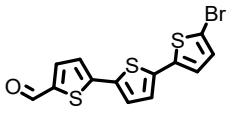


PTI-3

[**13**] (20 mg, 0.03 mmol, 1.0 eq) and lead (IV) oxide (36 mg, 0.15 mmol, 5.0 eq) were charged in a 50 mL of two neck flask with 10 mL of dichloromethane. The mixture was stirred at room temperature for 30 min. After stirring the reaction mixture at room temperature for 25 minutes the excess lead oxide was filtered off and the solvent was removed under reduced pressure to give **PTI-3** as a black solid (15 mg, 75%). HRMS (ESI$^+$): calcd. for $C_{41}H_{36}N_2OS_3$ 668.1990, found [M+H]$^+$ 671.2211(HRMS used methanol as solvent, so the sample may be reduced to [**13**] by methanol). Maldi-Tof mass spectrum found [M]$^+$ 667.97.

2.5 Synthesis of PTI-4

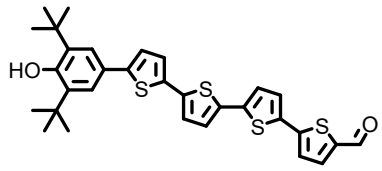
Synthesis of 16



16

5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophene-2-carbaldehyde[**14**] (2.00 g, 8.40 mmol, 1.0 eq), 5,5'-dibromo-2,2'-bithiophene[**15**] (2.72 g, 8.40 mmol, 1.0 eq), tetrakis(triphenylphosphine)palladium(0) (485 mg, 0.05 eq) and sodium carbonate (7.123 g, 67.2 mmol, 8.0 eq) were charged in a 250 mL of two neck flask with 35 mL of water and 70 mL of tetrahydrofuran under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 250 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 100 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The product was purified by column chromatography (SiO_2, hexane/DCM, V/V = 1: 1, as eluent) to give [**16**] as an orange solid (1576 mg, 53%).[3] MALDI-TOF m/z: [M]+ calcd. for $C_{13}H_7BrOS_3$ 353.88, found 353.89.

Synthesis of 17

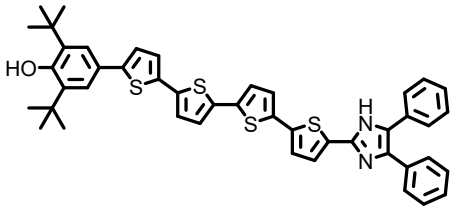


17

[**16**] (800 mg, 2.26 mmol, 1.0 eq), [**11**] (936 mg, 2.26 mmol, 1.0 eq), tetrakis(triphenylphosphine)palladium(0) (131 mg, 0.05 eq) and sodium carbonate (1.92 g, 18.08 mmol, 8.0 eq) were charged in a 100 mL of two neck flask with 9 mL of water and 18 mL of tetrahydrofuran under nitrogen. The mixture was heated to reflux for 16 h. The reaction was cooled down to room temperature and 80 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The product was purified by column chromatography (SiO_2, hexane/DCM, V/V = 1: 4, as eluent) to give [**17**] as an orange

solid (699 mg, 55%). ^{1}H NMR (400 MHz, DMSO-d6): δ = 9.89 (1 H, s), 8.00 (1 H, d, J_{HH} = 4 Hz), 7.59 (1 H, d, J_{HH} = 4 Hz), 7.56 (2 H, d, J_{HH} = 8 Hz), 7.40 (4 H, m), 7.32 (1 H, d, J_{HH} = 4 Hz), 7.13 (1 H, m), 5.75 (1 H, s), 1.42 (CH_3, 18 H, s). (Due to poor solubility, no carbon spectrum was obtained) MALDI-TOF m/z: [M]+ calcd. for $C_{31}H_{30}O_2S_4$ 562.11, found 562.05.

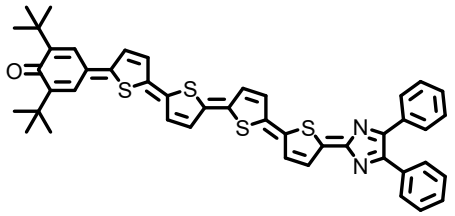
Synthesis of 18



18

Compound **17** (300 mg, 0.53 mmol, 1.0 eq), benzil (112 mg, 0.53 mmol, 1.0 eq) and ammonium acetate (368 mg, 4.77 mmol, 9.0 eq) were charged in a 100 mL of two neck flask with 30 mL of acetic acid under nitrogen. The mixture was shielded from light and heated to reflux for 16 h. The reaction was cooled down to room temperature and 150 mL of water was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. Hot dichloromethane was added to the residue until it just dissolved and then recrystallized in -20 ℃ to give [**18**] as an orange solid (243 mg, 61%). ^{1}H NMR (400 MHz, DMSO-d6): δ = 12.93 (1 H, s), 7.65 (1 H, d, J_{HH} = 4 Hz), 7.50 (4 H, d, J_{HH} = 8 Hz), 7.38 (4 H, m), 7.33 (1 H, s), 7.32 (2 H, m), 7.31 (1 H, m), 7.26 (1 H, s), 5.76 (1 H, s), 1.43 (CH_3, 18 H, s). (Due to poor solubility, no carbon spectrum was obtained) HRMS (ESI^+): calcd. for $C_{45}H_{40}N_2OS_4$ 752.2023, found $[M+H]^+$ 753.2097.

Synthesis of PTI-4



PTI-4

[**18**] (20 mg, 0.027 mmol, 1.0 eq) and lead (IV) oxide (32 mg, 0.135 mmol, 5.0 eq) were charged in a 50 mL of two neck flask with 10 mL of dichloromethane. The mixture was stirred at room temperature for 30 min. After stirring the reaction mixture at room temperature for 15 minutes the excess lead oxide was filtered off and the solvent was removed under reduced pressure to give **PTI-4** as a black solid (15 mg, 75%). HRMS (ESI^+): calcd. for $C_{41}H_{36}N_2OS_3$ 750.1867, found $[M+H]^+$ 751.1935. Maldi-Tof mass spectrum found $[M]^+$ 749.70.

3. NMR and Mass spectra

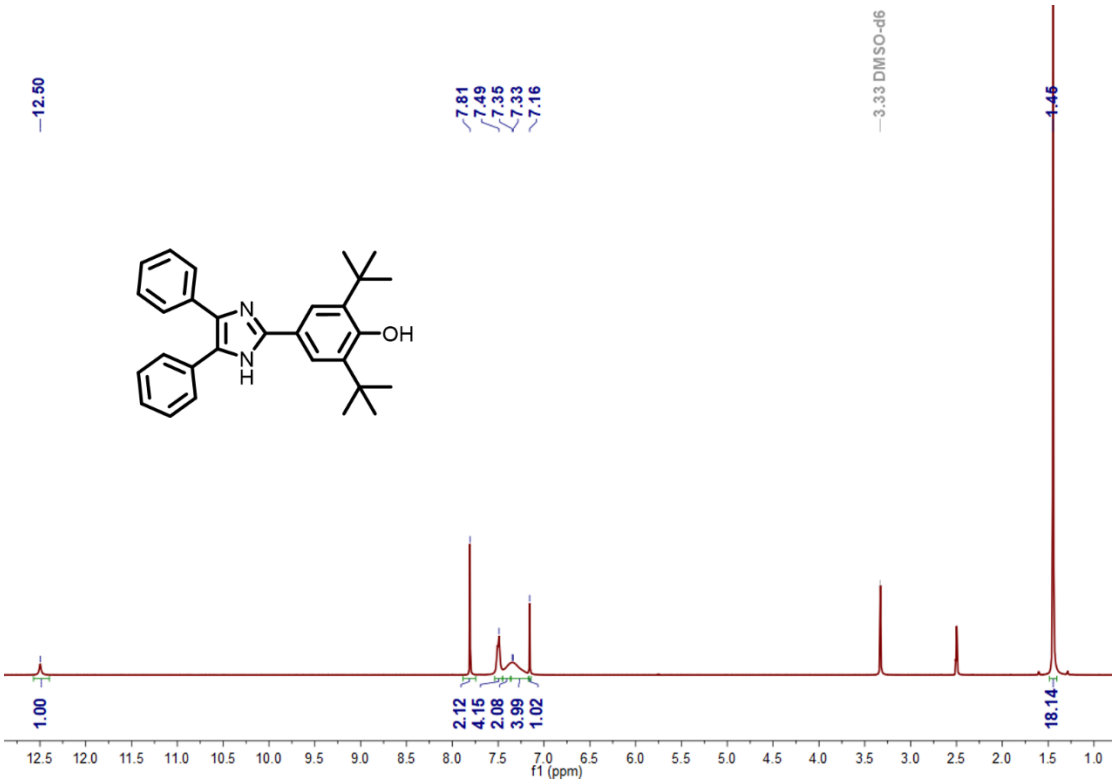


Figure S1. ^{1}H NMR spectrum of **2**.

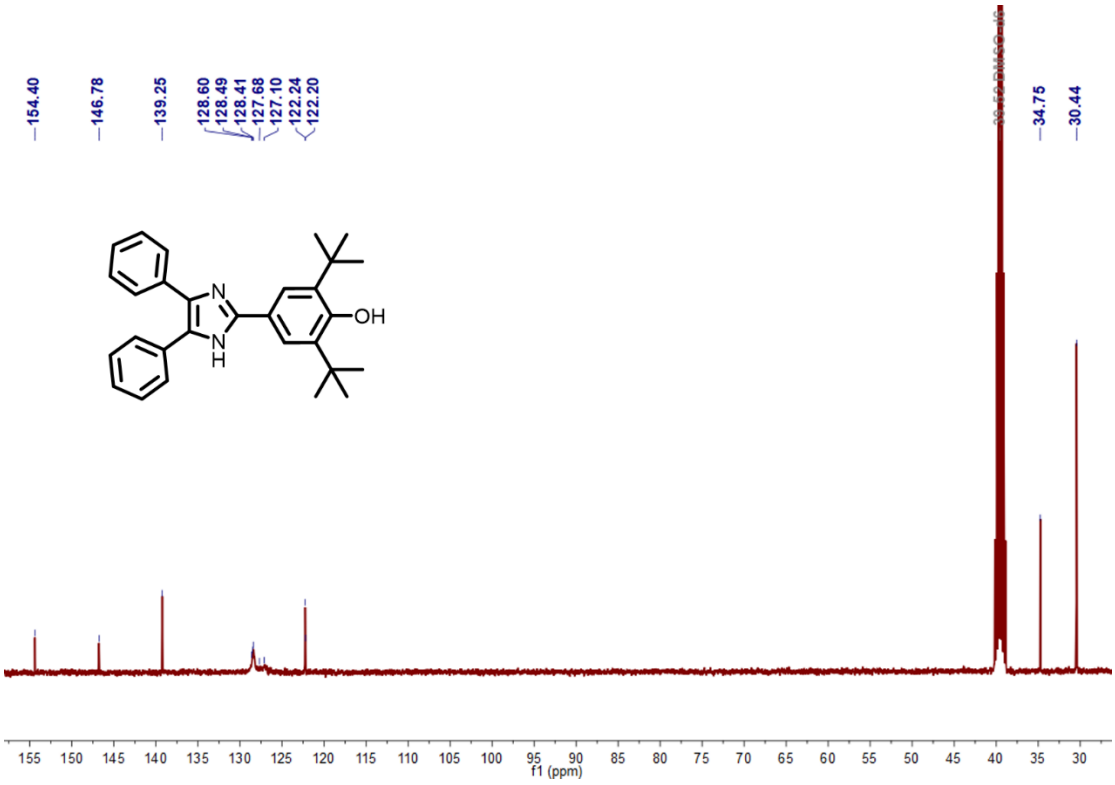


Figure S2. ^{13}C NMR spectrum of **2**.

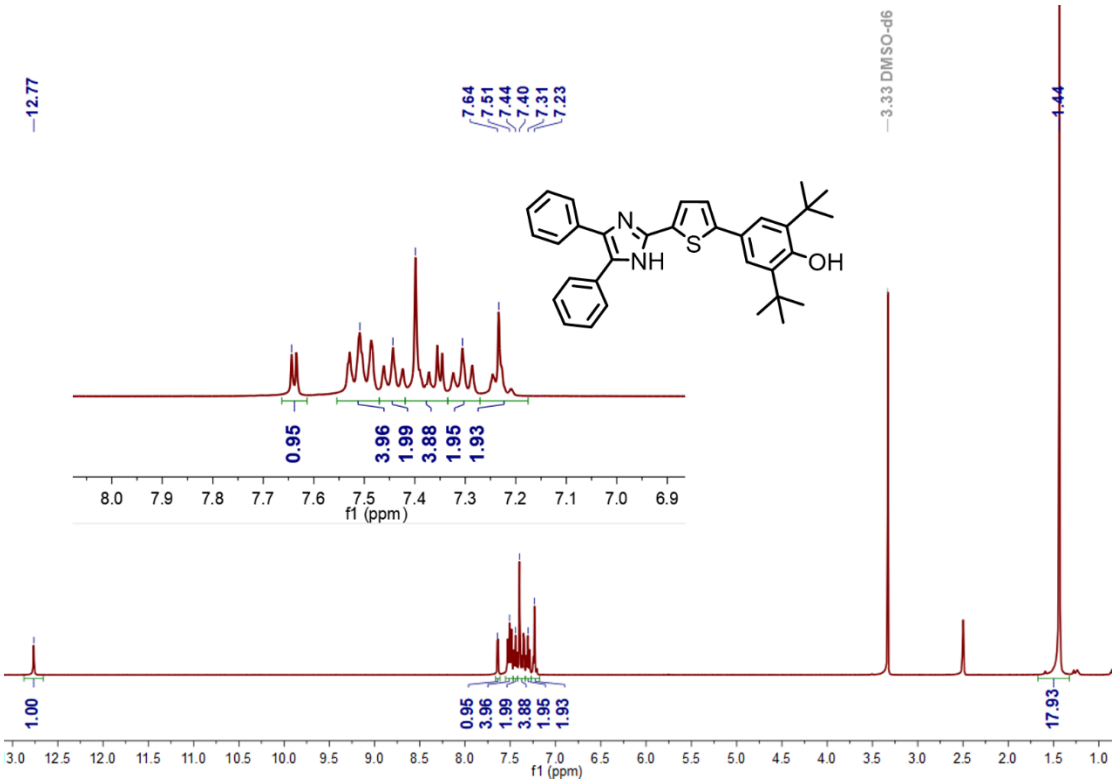


Figure S3. ^{1}H NMR spectrum of **5**.

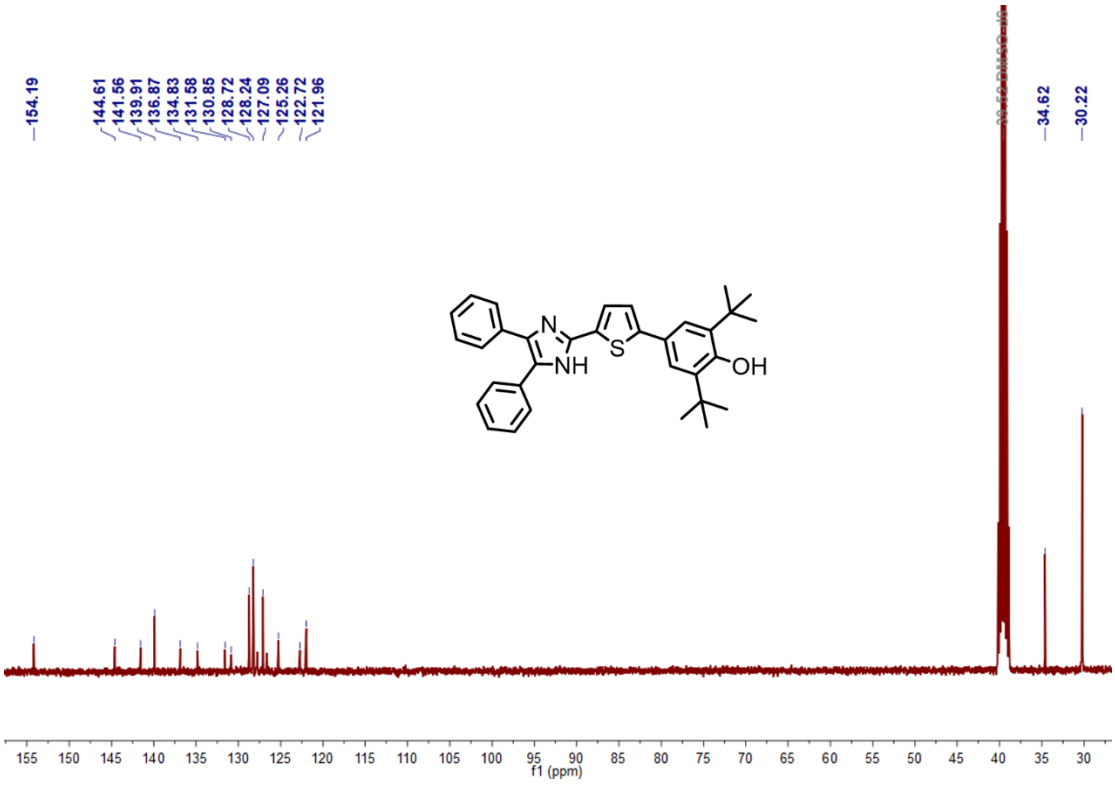


Figure S4. ^{13}C NMR spectrum of **5**.

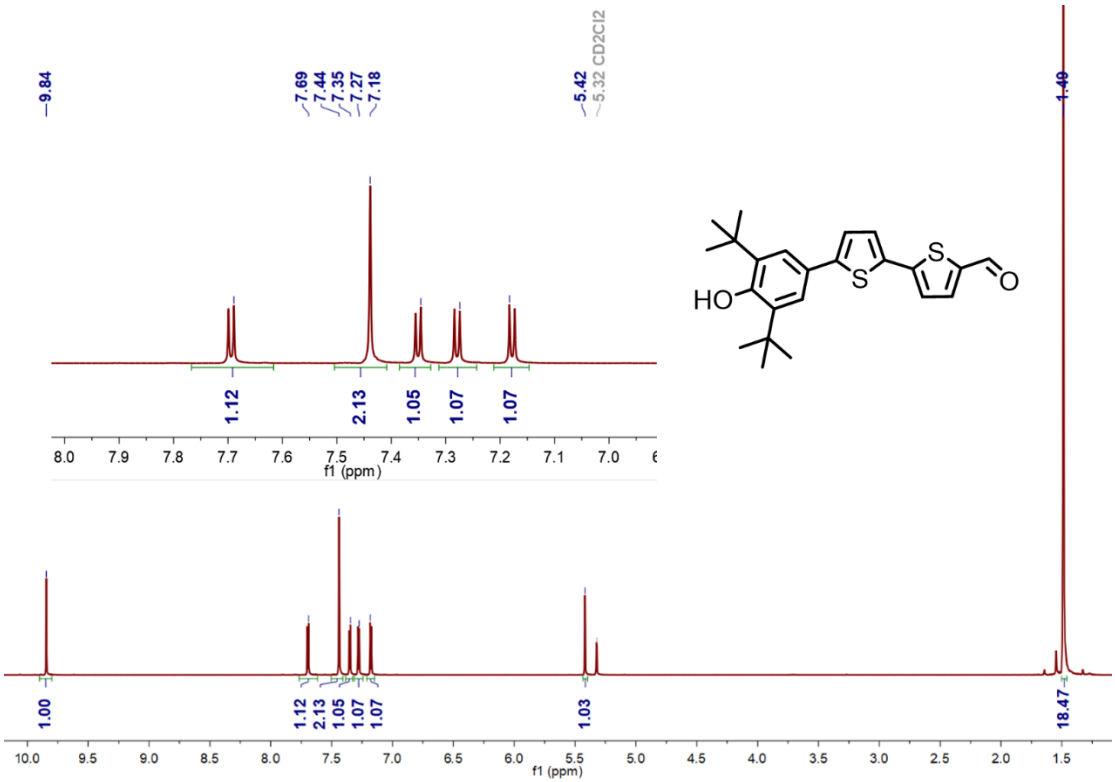


Figure S5. ^{1}H NMR spectrum of **8**.

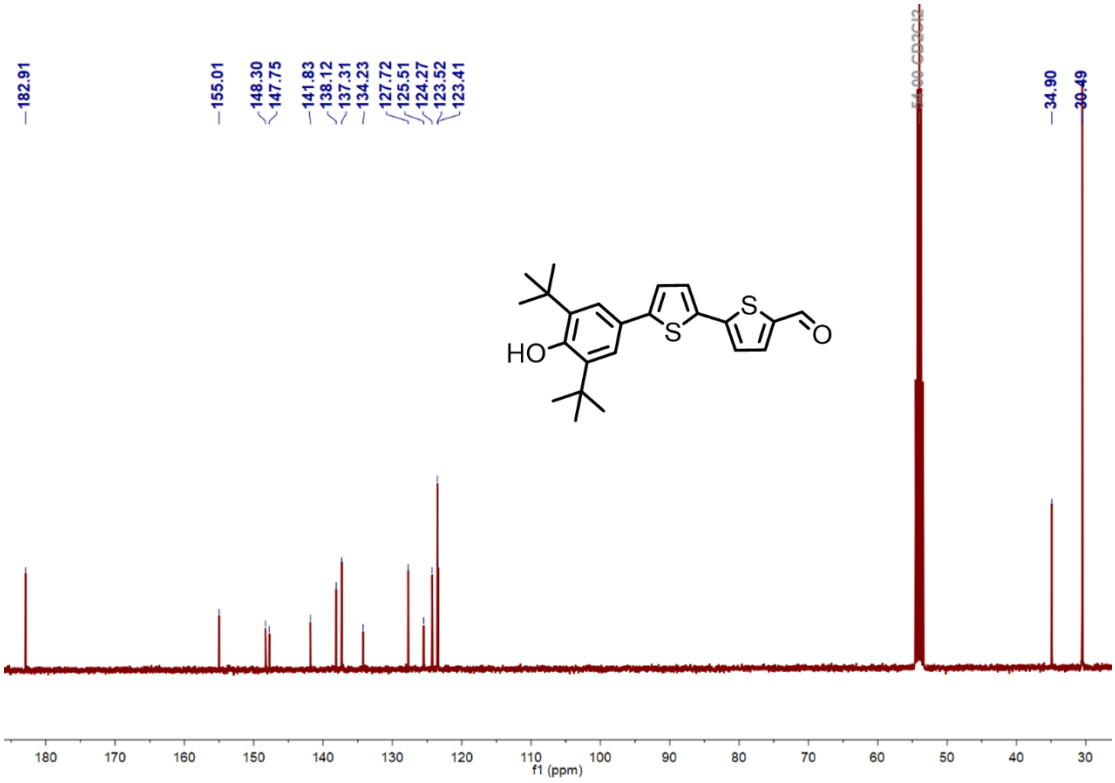


Figure S6. ^{13}C NMR spectrum of **8**.

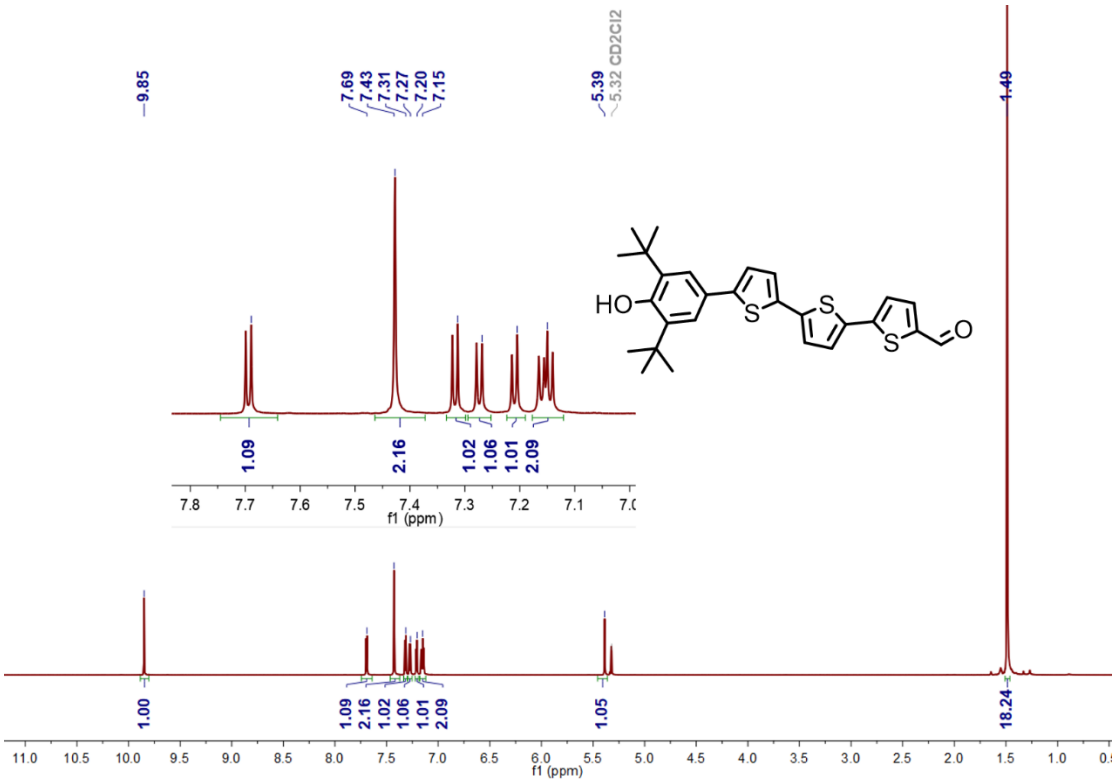


Figure S7. ^{1}H NMR spectrum of **12**.

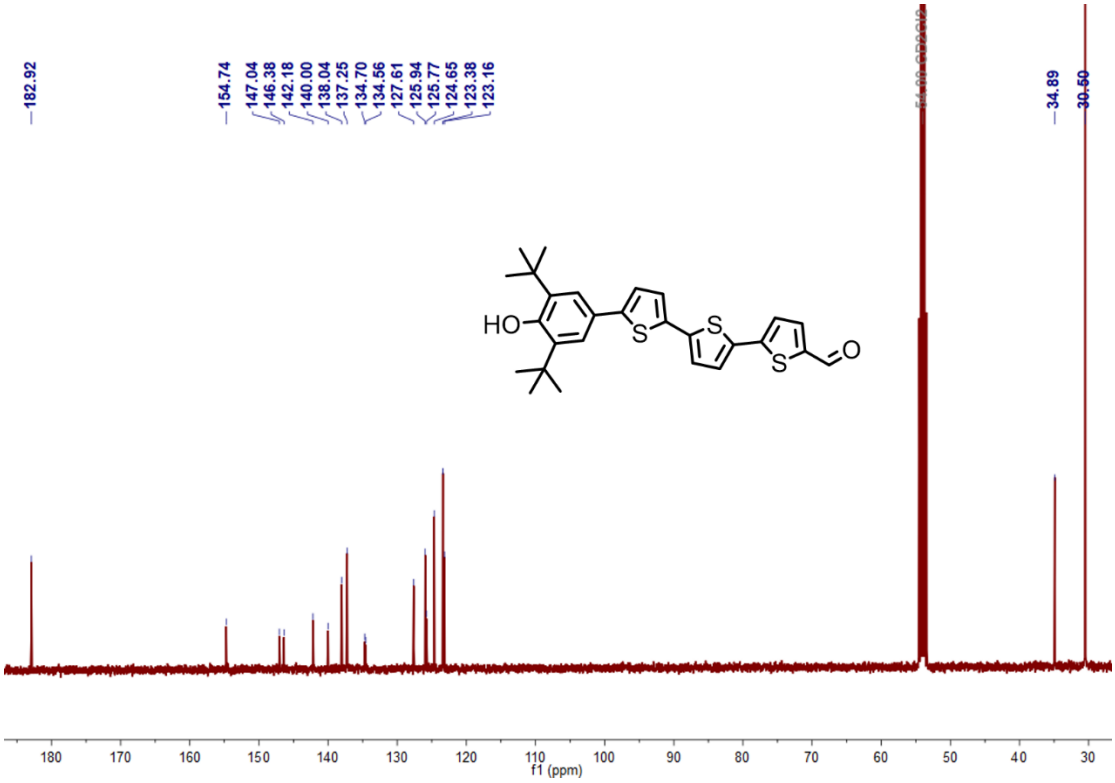


Figure S8. ^{13}C NMR spectrum of **12**.

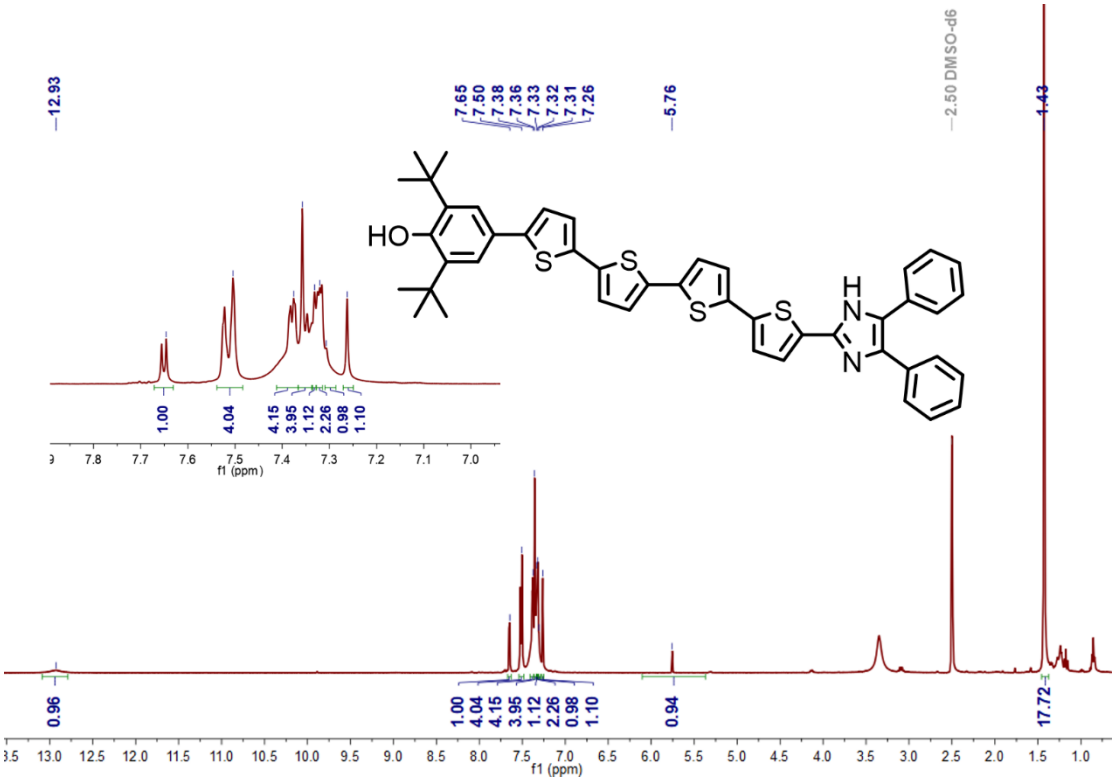


Figure S9. ^{1}H NMR spectrum of **17**.

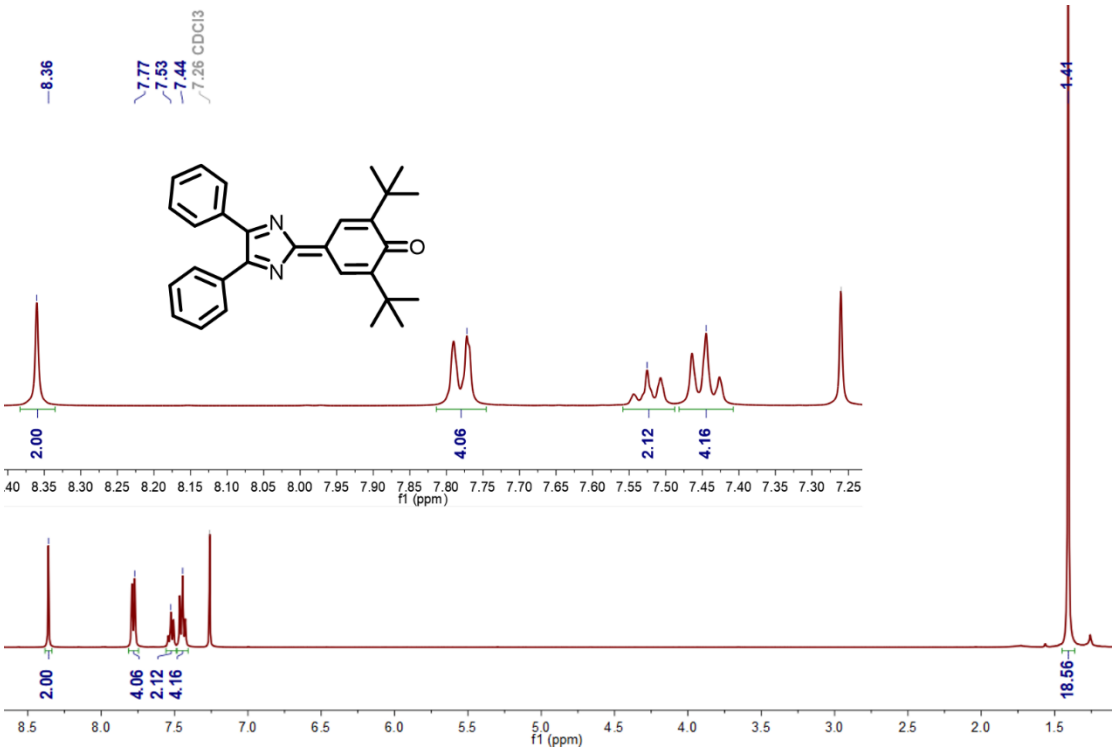


Figure S10. ^{1}H NMR spectrum of **PTI-0**.

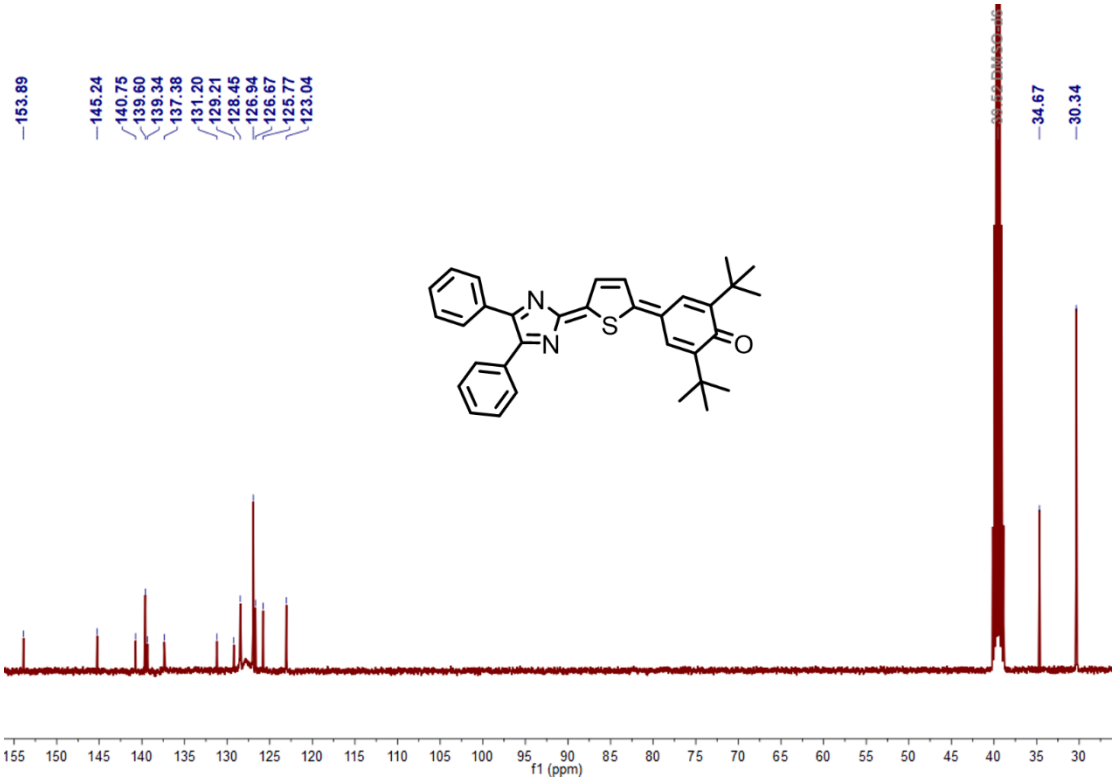


Figure S11. ^{13}C NMR spectrum of **PTI-0**.

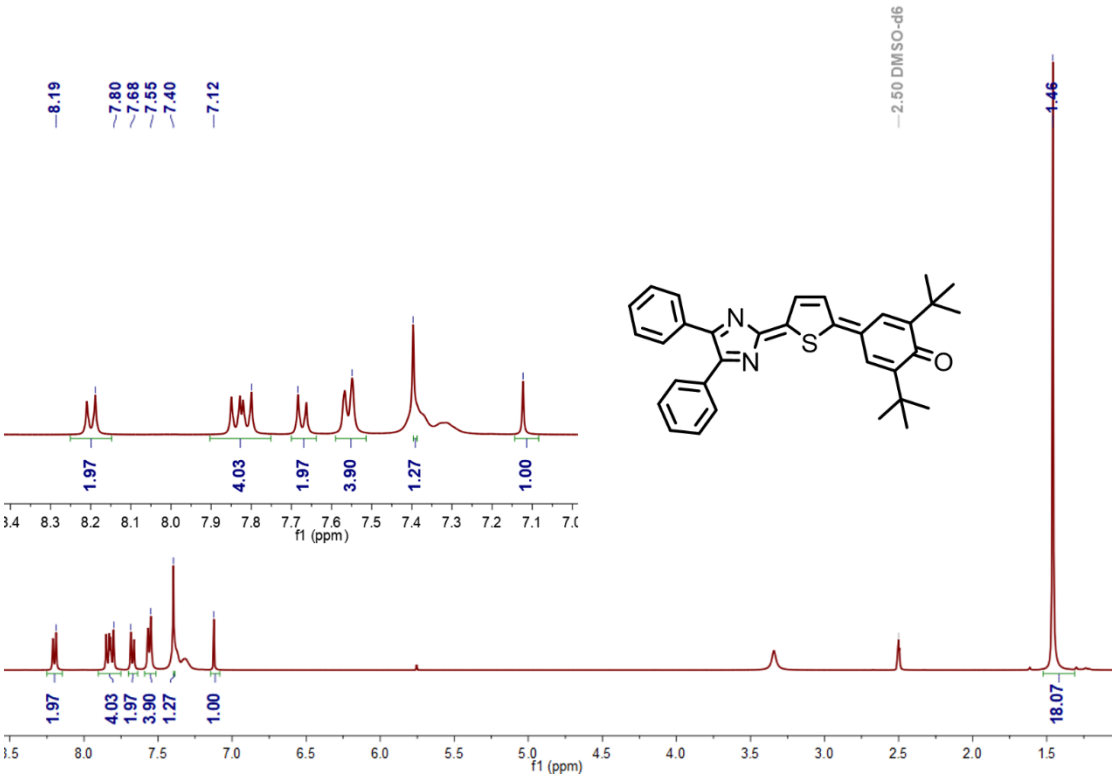


Figure S12. ^{1}H NMR spectrum of **PTI-1**.

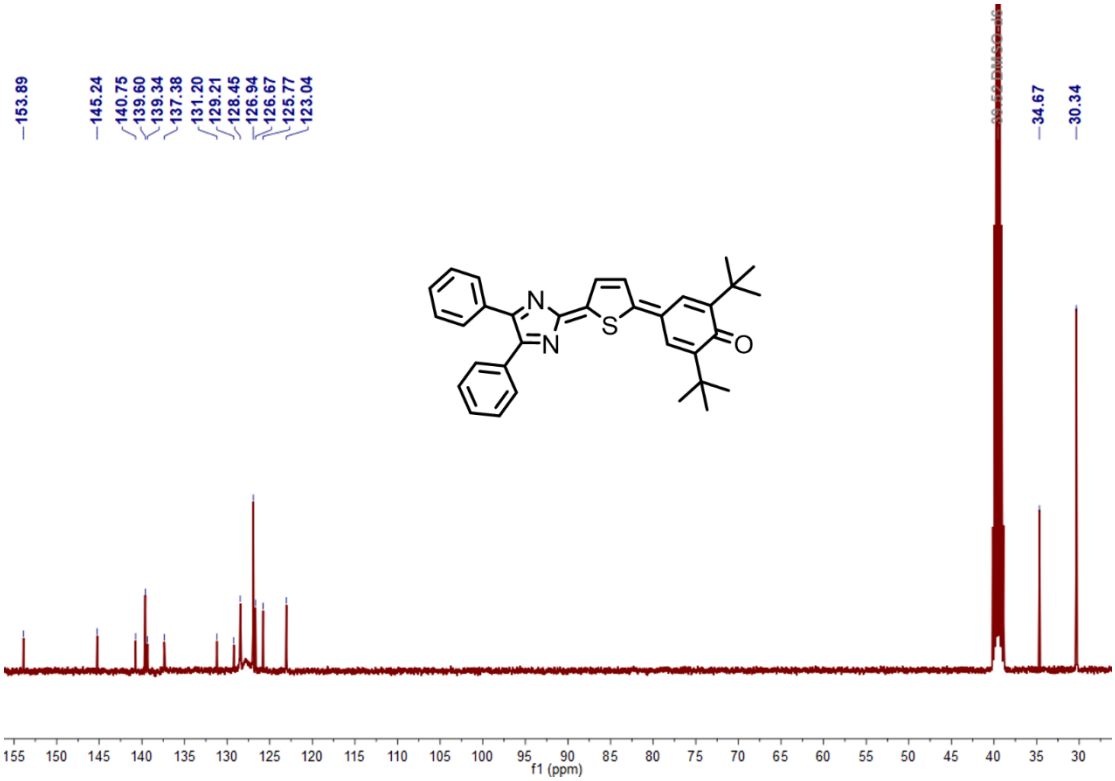


Figure S13. ^{13}C NMR spectrum of **PTI-0**.

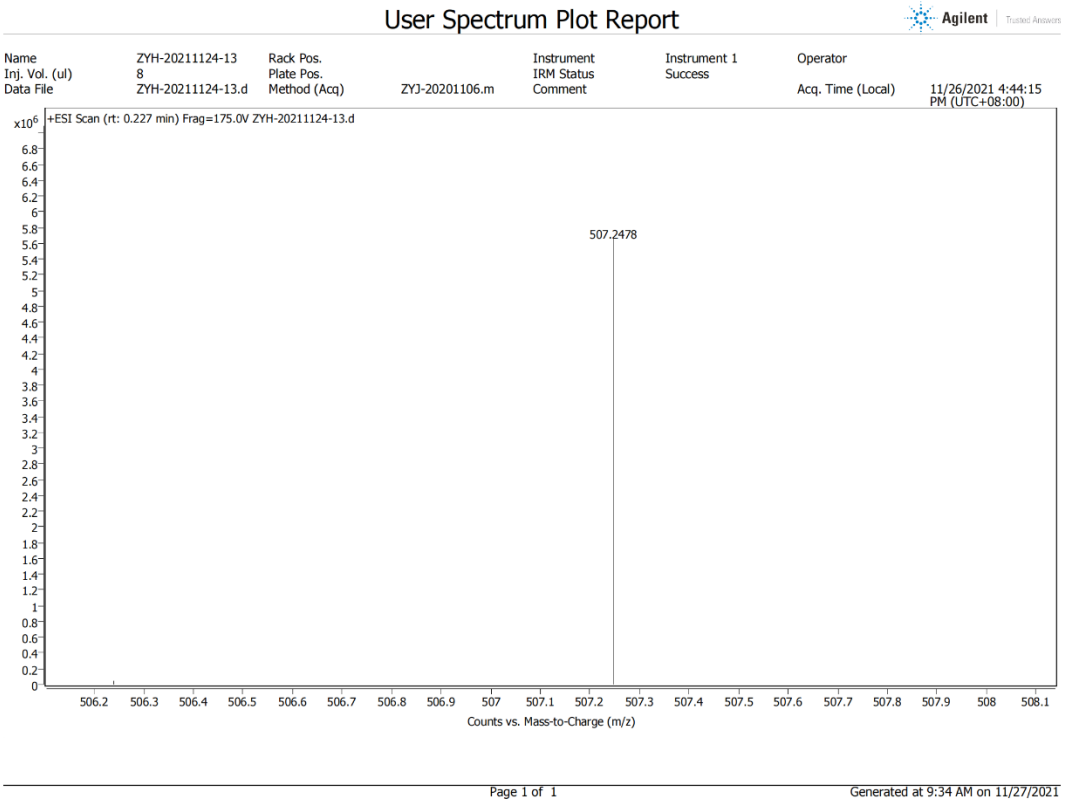


Figure S14. HR mass spectra of **5**.

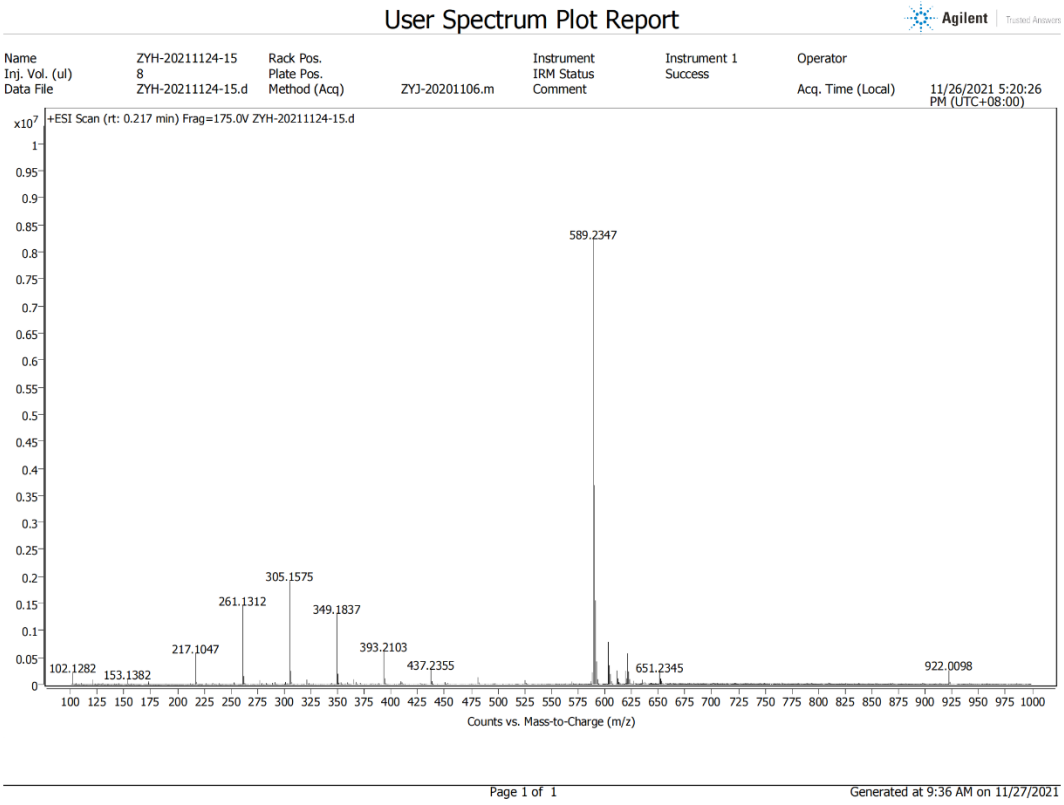


Figure S15. HR mass spectra of **9**.

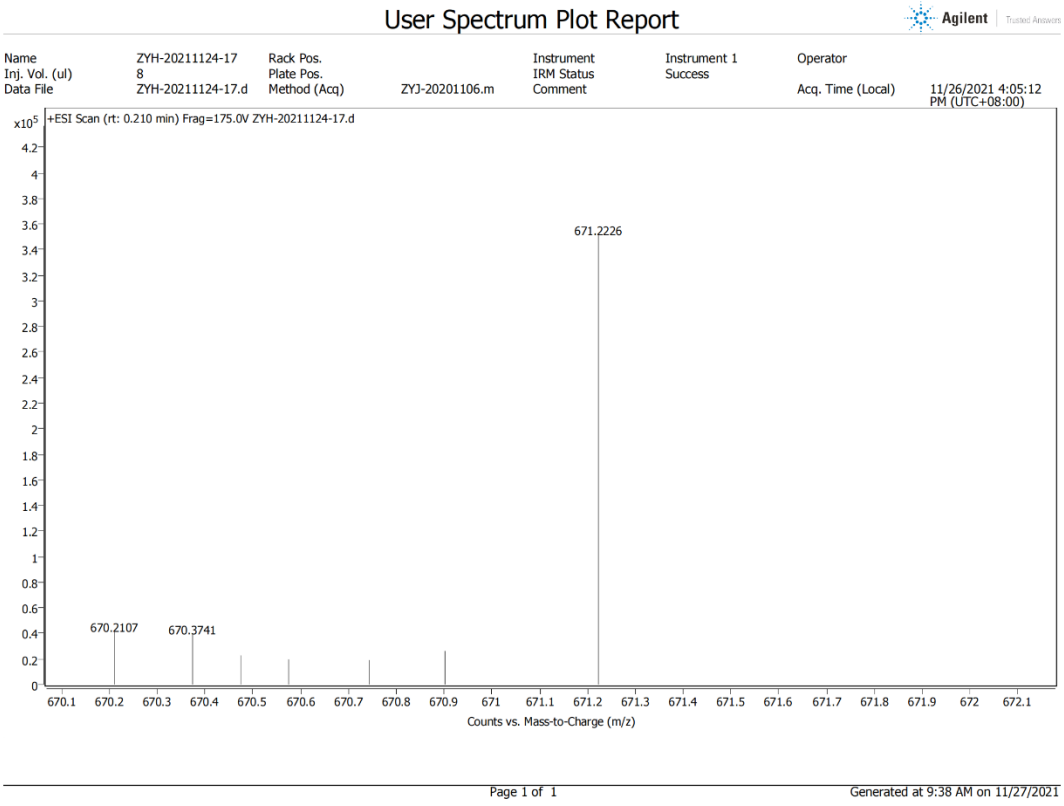


Figure S16. HR mass spectra of **13**.

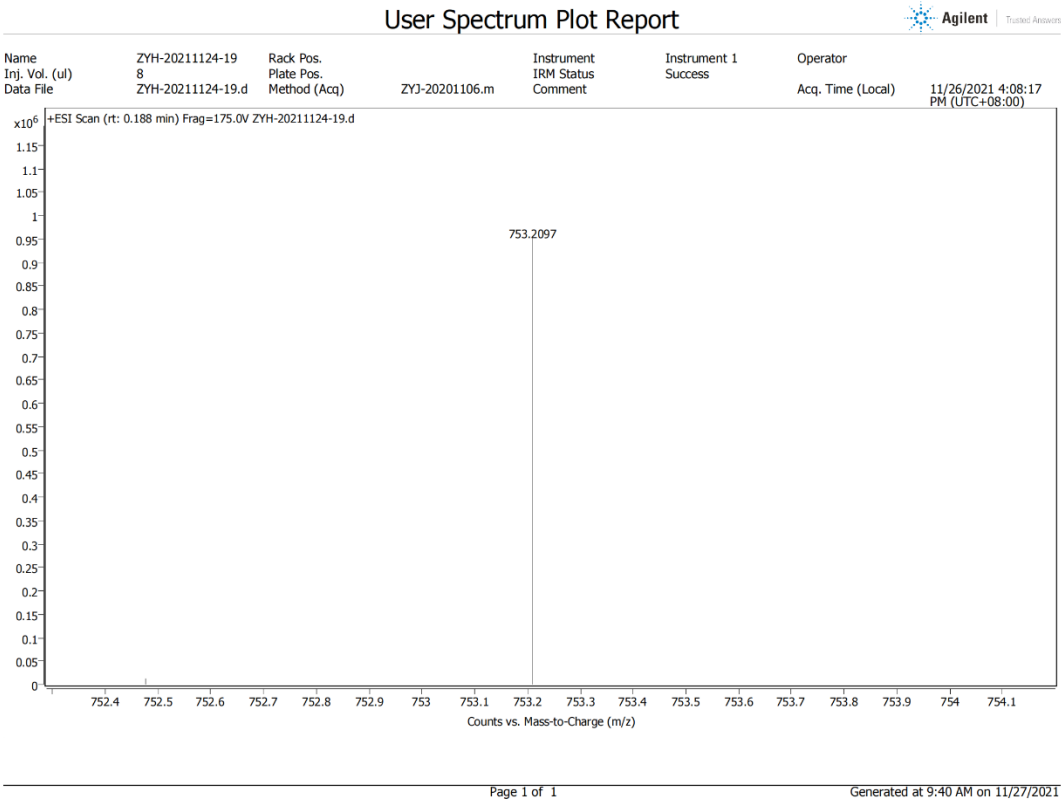


Figure S17. HR mass spectra of **18**.

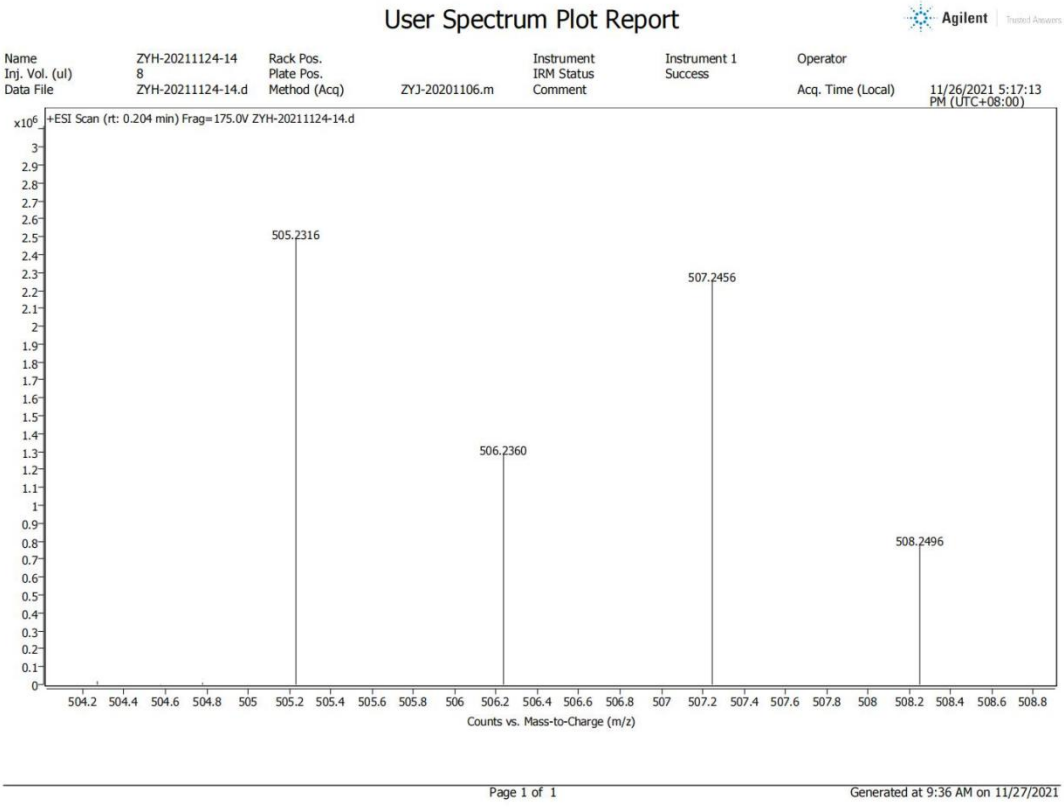


Figure S18. HR mass spectra of **PTI-1**.

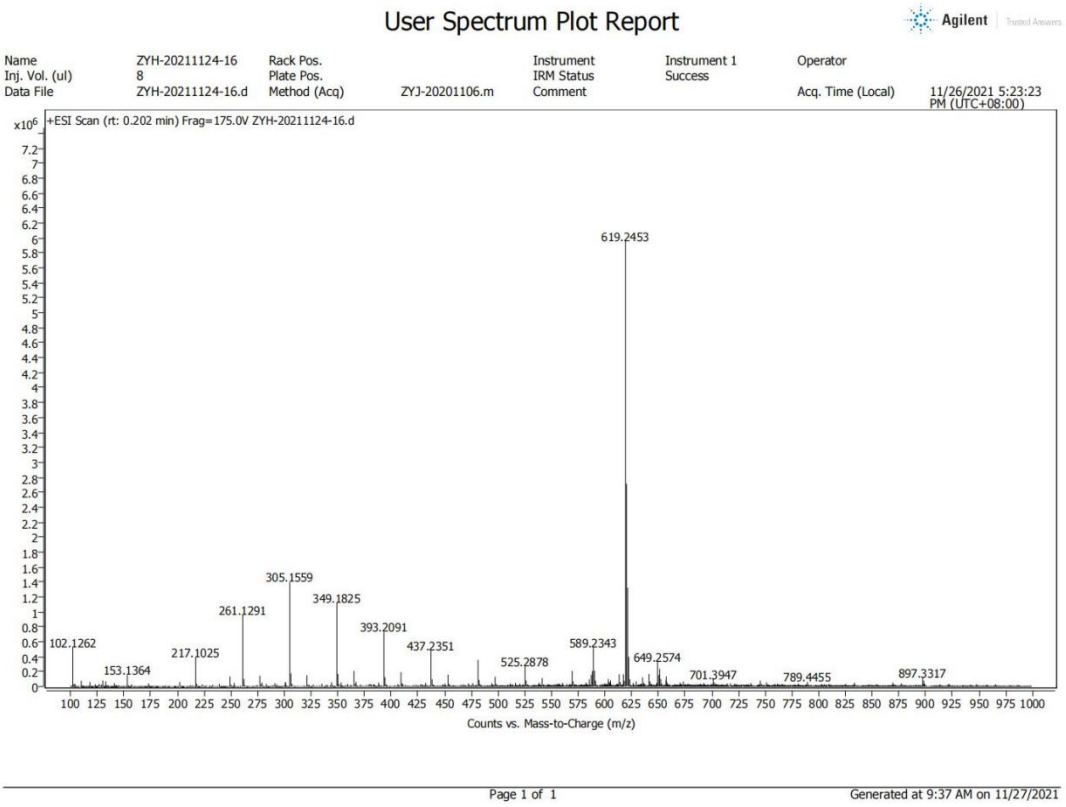


Figure S19. HR mass spectra of **PTI-2**.

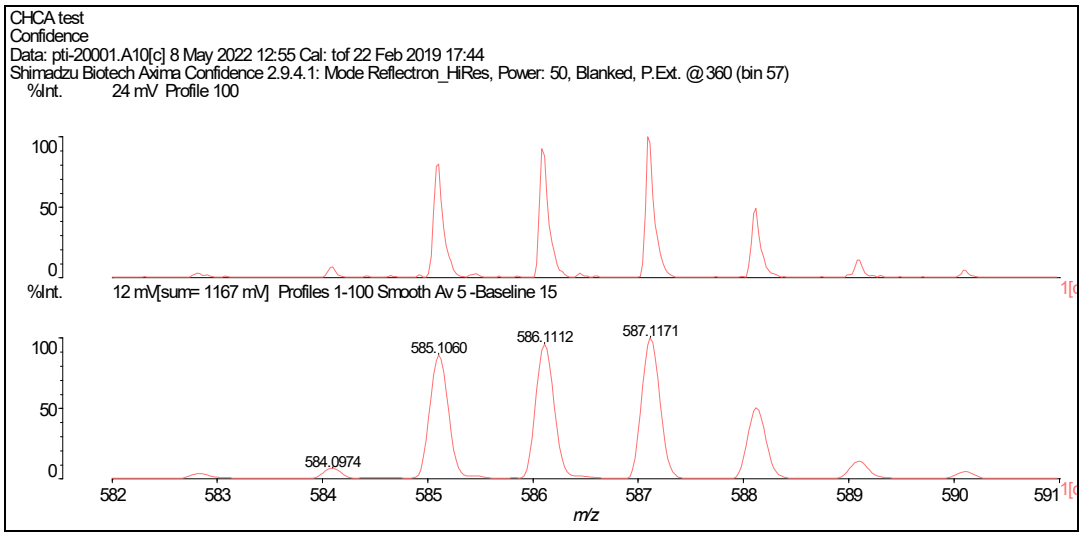


Figure S20. Maldi-Tof mass spectra of **PTI-2**.

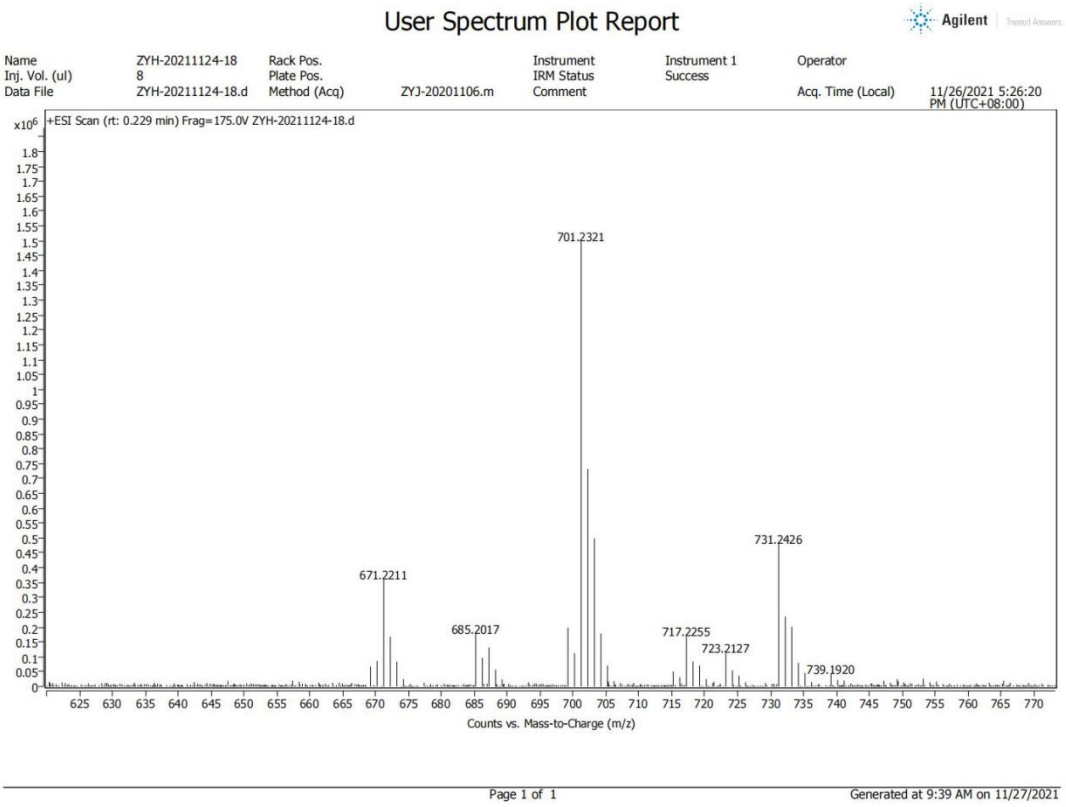


Figure S21. HR mass spectra of **PTI-3**.

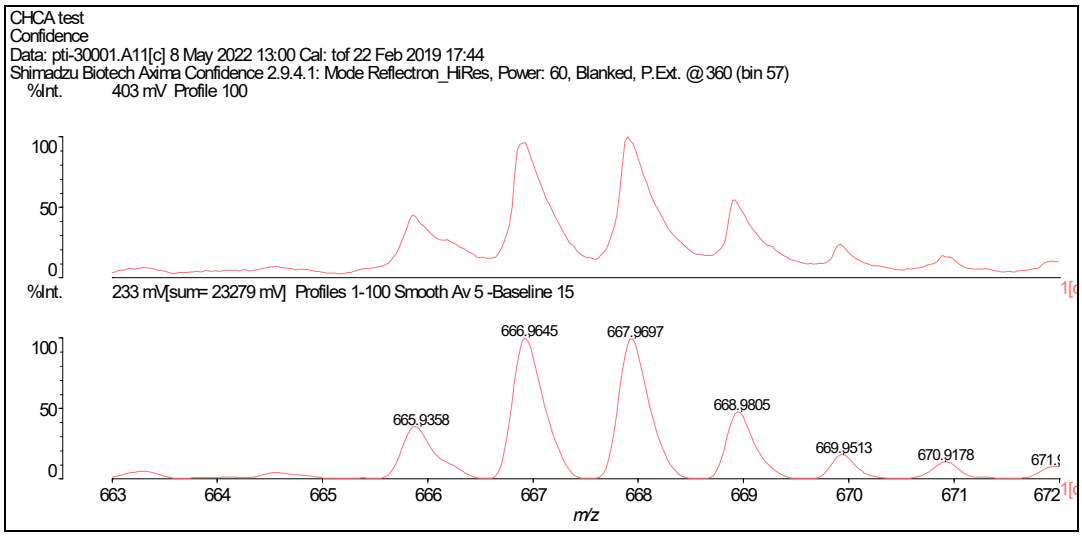


Figure S22. Maldi-Tof mass spectra of **PTI-3**.

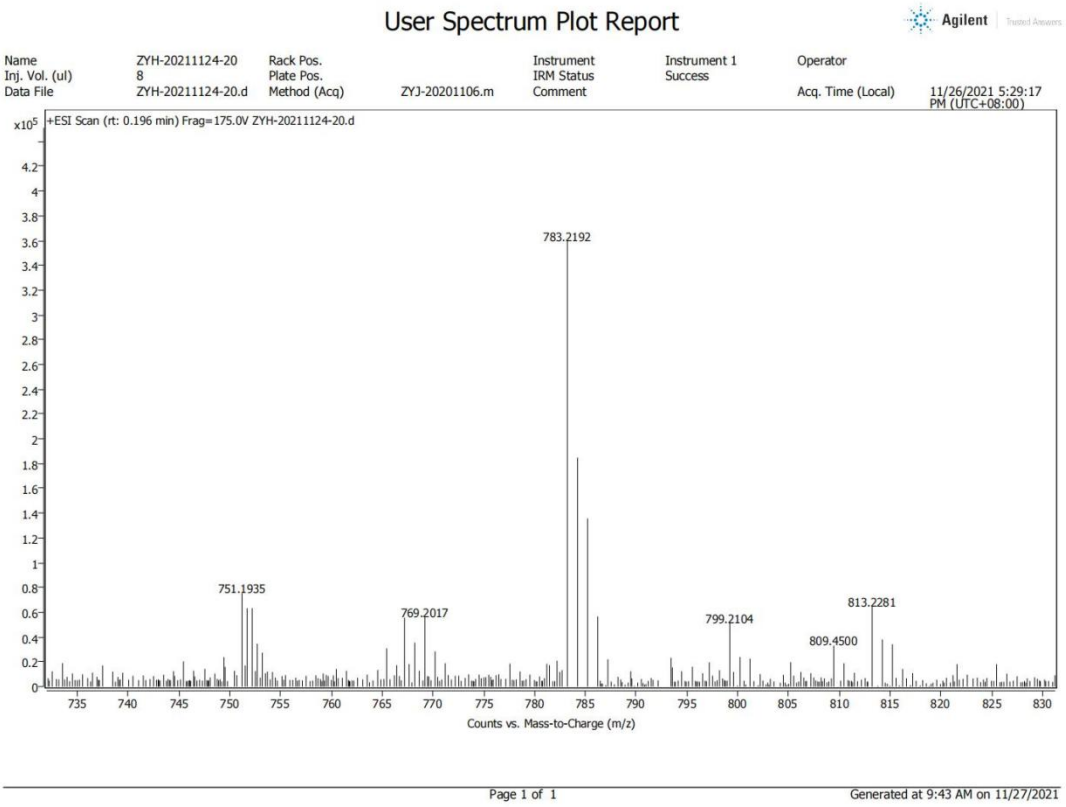


Figure S23. HR mass spectra of **PTI-4**.

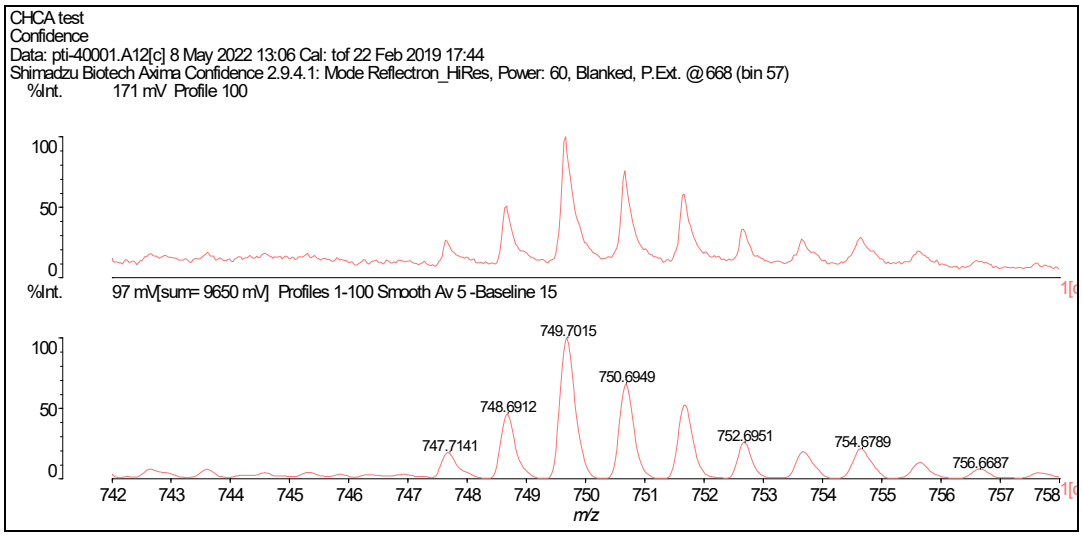


Figure S24. Maldi-Tof mass spectra of **PTI-4**.

4. Reaction progress of PTI-3 and PTI-4

PTI-3 and **PTI-4** completed reaction in 25 and 15 min, respectively.

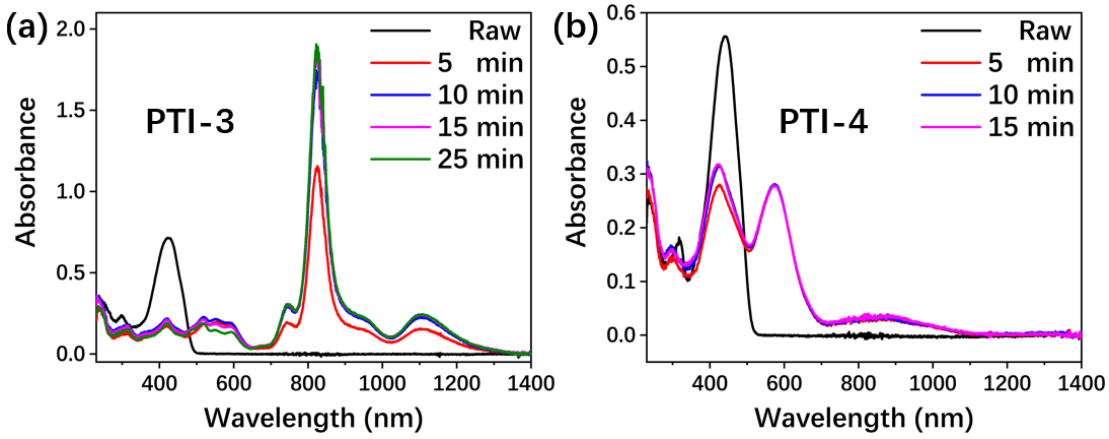


Figure S25. The UV/vis/NIR absorption spectra in reaction progress of **PTI-3**(a) and **PTI-4**(b) in dry DCM with concentration of 10^{-4} mol/L.

5. Optical energy gap

UV/vis/NIR absorption spectra (Figure S26) revealed that the absorption onsets were 499, 705, 971, 1279 and 1112 nm for **PTI-0**, **1**, **2**, **3**, **4** respectively. The corresponding optical energy gaps E_g^{Opt} are 2.48, 1.76, 1.28, 0.97 and 1.12 eV for **PTI-0**, **1**, **2**, **3**, **4** respectively.

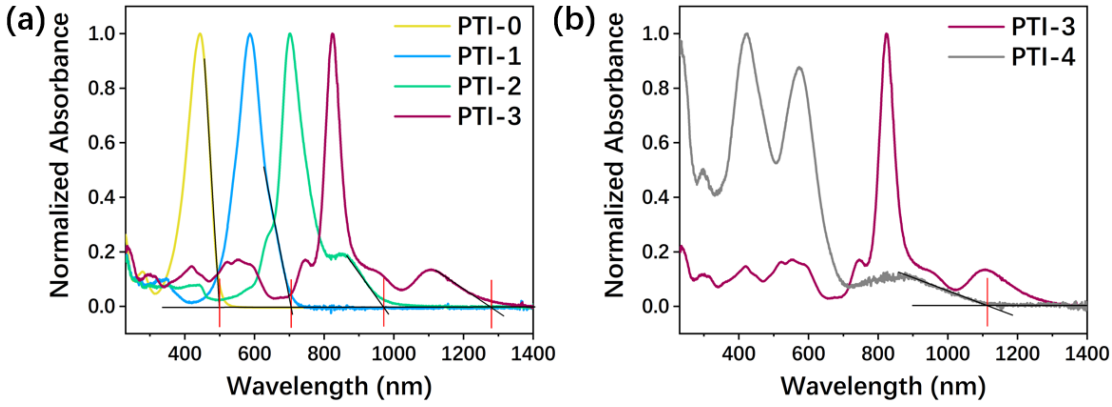


Figure S26. The UV/vis/NIR absorption spectra of **PTI-n** in dry DCM.

6. VT ESR measurement

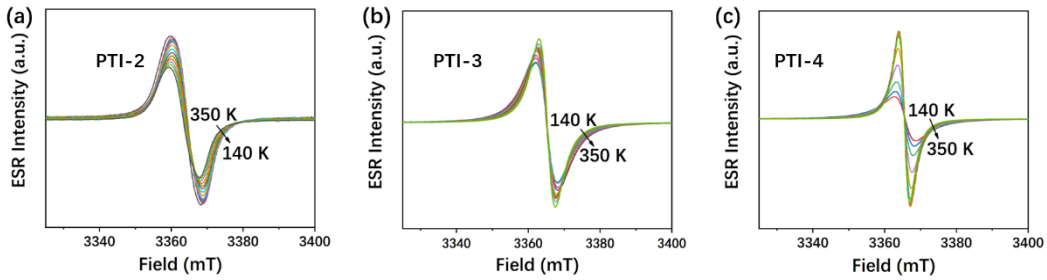


Figure S27. Variable-temperature ESR measurements in solid from 140 to 350 K of **PTI-2** (a), **PTI-3** (b) and **PTI-4** (c).

7. X-ray single crystal data

Table S1. Sample and crystal data for **PTI-1** (CCDC Number: 2169134)

Chemical formula	$C_{34}H_{36}N_2O_2S$	
Formula weight	536.71 g/mol	
Temperature	156 K	
Wavelength	1.34139 Å	
Space group	P -1	
Unit cell dimensions	a = 13.680(5) Å	α = 70.396(13) °
	b = 14.852(5) Å	β = 69.946(15) °
	c = 16.684(6) Å	γ = 86.860(15) °
Volume	2987.3(18) Å^3	
Z	4	
Density (calculated)	1.193 g/cm^3	
Absorption coefficient	0.785 mm^{-1}	
F(000)	1144	

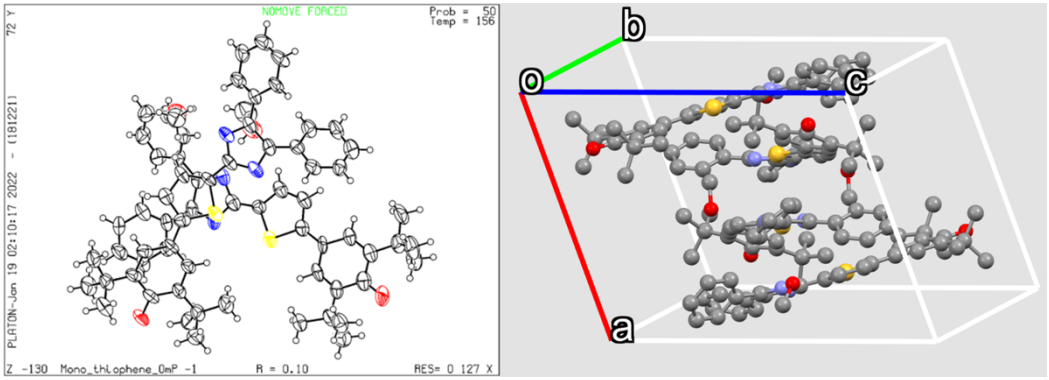


Figure S28. Single crystal X-ray structure and Packing model of **PTI-1**

8. Computational details

Theoretical calculations were performed with the Gaussian16 program suite[4] using a supercomputer. All calculations were carried out using the density functional theory (DFT) method with Becke's three-parameter hybrid exchange functionals and the Lee-Yang-Parr correlation functional (B3LYP)[5-6] employing the 6-311G(d) basis set[7-9] for all atoms. Meanwhile, harmonic vibrational frequencies were calculated at the same level of optimization to guarantee that the optimized structures were local minima. Singlet biradical was calculated using a symmetry-broken UB3LYP/6-311G(d) method along with geometry optimization. The singlet biradical index y_0 was determined on the basis of the LUMO occupation number. A perfect biradical is characterized by occupation numbers of 1.0 in HOMO and LUMO (y_0=1), whereas a perfect closed-shell molecule possesses occupation numbers of 2.0 and 0.0 in HOMO and LUMO (y_0=0), respectively[10]. The spin densities and frontier molecular orbitals were illustrated using Multiwfn[11] and VMD[12]. To simulate the ground-state absorption spectra, the time-dependent (TD) DFT calculation was employed with UB3LYP/6-311G(d) level. The Cartesian coordinates for all atoms of optimized geometries are attached at the end of this Supporting Information.

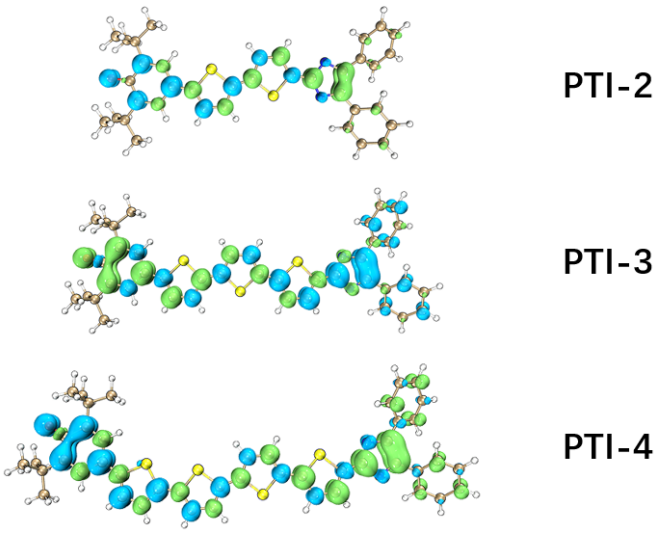


Fig. S29 Calculated (UB3LYP) spin density distribution of **PTI-2**, **PTI-3** and **PTI-4**. Blue and green surfaces represent α and β spin densities, respectively. Isovalue is 0.001.

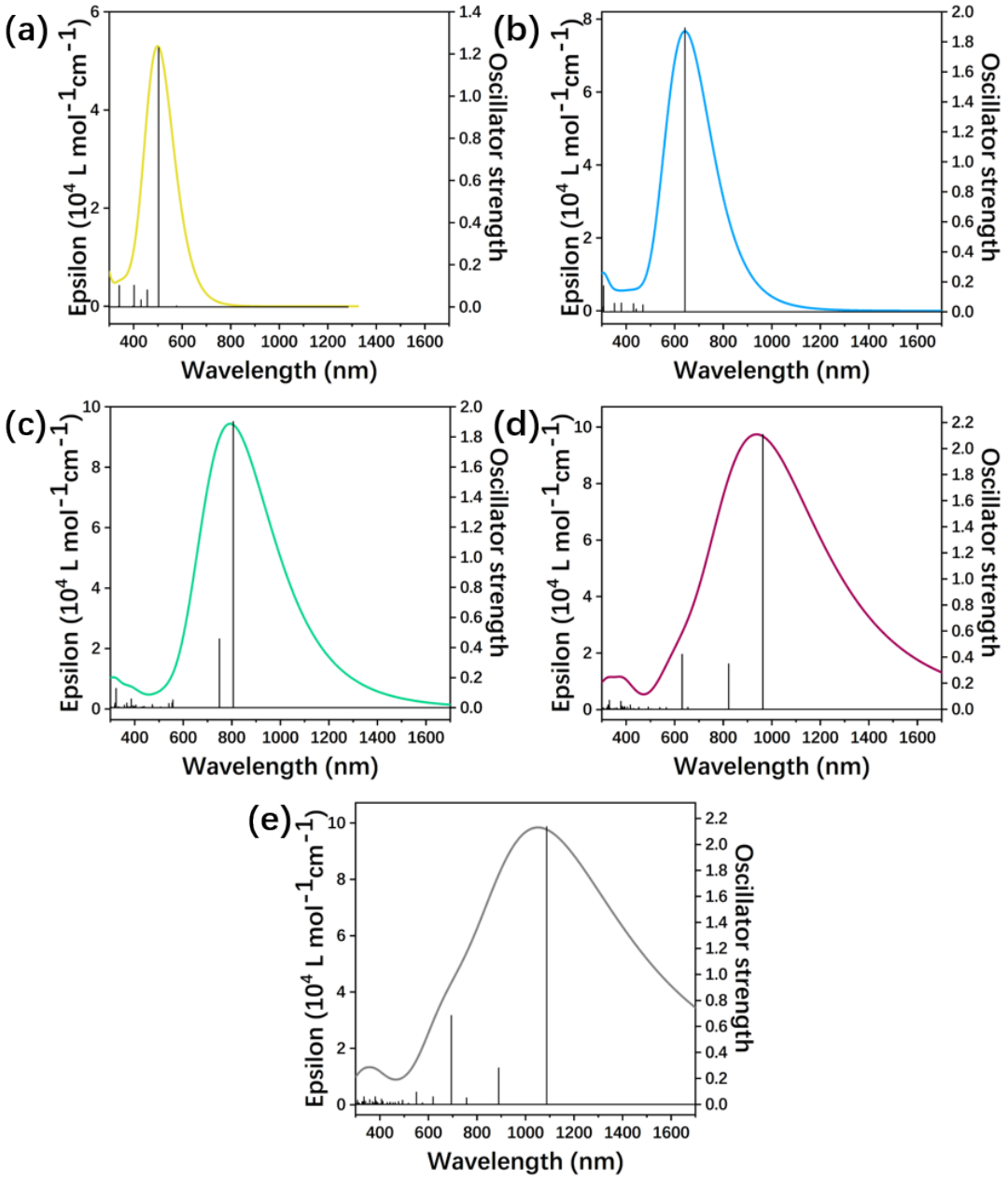


Figure S30. TD-DFT calculated absorption spectra of (a) **PTI-0**, singlet; (b) **PTI-1**, singlet; (c) **PTI-2**, singlet; (d) **PTI-3**, singlet; (e) **PTI-4**, singlet.

Table S2. Calculated absorption and Oscillator strength for **PTI-n**.

PTI-0 (singlet)		
Wavelength (nm)	Oscillator strength	Major contributions
503.06	1.2300	Hb → Lb 47.5%, Ha → La 47.5%

456.45	0.0809	Hb-2 -> Lb 47.1%, Ha-2 -> La 47.1%
401.98	0.1033	Hb-6 -> Lb 21.3%, Ha-6 -> La 21.3% Ha-7 -> La 19.1%, Hb-7 -> Lb 19.1% Ha-3 -> La 7.7%, Hb-3 -> Lb 7.7%
341.06	0.1020	Hb-7 -> Lb 26.1%, Ha-7 -> La 26.1% Ha-6 -> La 20.7%, Hb-6 -> Lb 20.7%
231.88	0.2052	Hb-2 -> Lb+1 22.8%, Ha-2 -> La+1 22.8% Hb-16 -> Lb 14.3%, Ha-16 -> La 14.3%

PTI-1 (singlet)

Wavelength (nm)	Oscillator strength	Major contributions
642.44	1.8938	Hb -> Lb 50.9%, Ha -> La 50.9%
469.44	0.0473	Ha-2 -> La 49.2%, Hb-2 -> Lb 49.2%
430.17	0.0548	Hb-6 -> Lb 32.0%, Ha-6 -> La 32.0% Ha-3 -> La 9.9%, Hb-3 -> Lb 9.9%
380.38	0.0592	Hb-8 -> Lb 45.5%, Ha-8 -> La 45.5%
352.03	0.0568	Hb -> Lb+1 26.4%, Ha -> La+1 26.4% Ha-9 -> La 10.4%, Hb-9 -> Lb 10.4% Ha-3 -> La 7.5%, Hb-3 -> Lb 7.5%
307.29	0.1735	Ha -> La+2 38.3%, Hb -> Lb+2 38.3% Ha-9 -> La 8.2%, Hb-9 -> Lb 8.2%

PTI-2 (singlet)

Wavelength (nm)	Oscillator strength	Major contributions
805.56	1.9020	Hb -> Lb 41.0%, Ha -> La 37.2% Hb-1 -> Lb 11.3%, Ha-1 -> La 7.3%

748.43	0.4571	Ha-1 -> La 29.5%, Hb-1 -> Lb 27.2% Ha -> La 15.8%, Hb -> Lb 9.7% Ha -> La+1 7.9%, Hb -> Lb+1 7.2%
557.41	0.0519	Ha-2 → La 22.6%, Hb-2 → Lb 22.6%, Ha → La+3 6.9%, Hb → Lb+3 6.9%
385.36	0.0582	Ha-8 -> La 58.3% Hb-9 -> Lb 13.7% Ha-1 -> La+1 6.8%
323.01	0.1281	Ha -> La+2 27.9% Hb -> Lb+3 31.1%, Ha -> La+3 13.5% Hb-13 -> Lb 9.3%
246.93	0.1296	Ha-10 -> La+1 19.4%, Hb-10 -> Lb+1 16.5% Ha-1 -> La+2 11.6%, Hb-1 -> Lb+2 10.6% Hb-9 -> Lb+1 7.8%, Ha-9 -> La+1 6.6%

PTI-3 (singlet)

Wavelength (nm)	Oscillator strength	Major contributions
962.91	2.1081	Hb -> Lb 41.4%, Ha -> La 35.8% Ha-1 -> La 11.0%, Hb-1 -> Lb 8.6%
822.18	0.3485	Ha-1 -> La 32.0%, Hb-1 -> Lb 27.4% Hb -> Lb 15.4%, Ha -> La 9.4% Hb -> Lb+1 8.1%, Ha -> La+1 6.2%
630.99	0.4225	Hb -> Lb+1 57.0%, Ha -> La+1 17.9% Hb-1 -> Lb 18.3%
330.81	0.0698	Ha-14 -> La 42.5% Hb -> Lb+3 20.7%, Ha -> La+3 9.9%

PTI-4 (singlet)		
Wavelength (nm)	Oscillator strength	Major contributions
1087.68	2.1363	Ha -> La 48.4%, Hb -> Lb 27.4% Hb-1 -> Lb 10.9%, Ha-1 -> La 9.9%
889.16	0.2810	Hb-1 -> Lb 37.2%, Ha-1 -> La 23.9% Ha -> La 16.0%, Hb -> Lb 8.4% Ha -> La+1 8.0%
694.28	0.6835	Ha -> La+1 56.1%, Hb -> Lb+1 19.9% Ha-1 -> La 14.0%
550.43	0.0955	Ha-1 -> La 23.6%, Hb-1 -> Lb 15.7% Ha -> La+1 16.3% Hb -> Lb+1 14.7% Ha-3 -> La 12.6%, Hb-3 -> Lb 12.5%

Table S3. $\Delta E_{S\text{-}T}$ and y of **PTP-n**, **PTI-n** and **ITI-n**

	$\triangle E_{s\text{-}t}$ [kcal/mol]			y		
n	PTP-n	PTI-n	ITI-n	PTP-n	PTI-n	ITI-n
2	-5.61	-5.67	-6.69	0.03	0.01	0.001
3	-2.42	-2.52	-2.19	0.28	0.25	0.05
4	-0.98	-1.20	-1.43	0.55	0.48	0.40

Table S4. Alpha-E_g and Beta-E_g of **PTP-n**, **PTI-n** and **ITI-n**

	Alpha-E_g [eV]			Beta-E_g [eV]		
n	PTP-n	PTI-n	ITI-n	PTP-n	PTI-n	ITI-n
2	-5.44	-5.35	-5.29	1.65	1.53	1.46
3	-5.33	-5.30	-5.16	1.55	1.49	1.36
4	-5.25	-5.15	-5.11	1.48	1.38	1.33

Table S5. Bond length of a, b, c and d in Figure 6.

n	a (Å)	b (Å)	c (Å)	d (Å)
1	1.3905	1.3910	1.3826	1.3822
2	1.4060	1.3946	1.3872	1.3870
3	1.4215	1.4214	1.4064	1.3906
4	1.4261	1.4252	1.4096	1.4086

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Cartesian coordinates for all atoms of optimized geometries (PTI-n)

PTI-1 in the singlet state (CS; rb3lyp/6-311g(d))

C	-1.62137000	-0.78022300	-0.00850800
C	-1.04745800	-2.09472400	-0.02457700
C	0.31405800	-2.11752500	-0.02747700
C	0.90761600	-0.82046100	-0.01291800
S	-0.31998000	0.42847600	0.00285300
C	2.26136700	-0.53972500	-0.00896700
C	-2.96925200	-0.43676300	-0.00312800
N	3.22255100	-1.53284900	-0.01093800
C	4.36578100	-0.88156800	0.00617200
C	4.07633000	0.57723800	-0.01450800
N	2.76909400	0.73923200	-0.00329400
C	5.64637800	-1.59767600	0.08056200
C	4.98376300	1.72841100	-0.08363700
C	6.73907300	-1.09614300	0.80504800
C	7.91889800	-1.82756600	0.90163100
C	8.03127100	-3.06580400	0.27255500
C	6.94899800	-3.57761800	-0.44412600
C	5.76563700	-2.85571300	-0.53326200
C	6.20805600	1.67374800	-0.76896100
C	7.01726200	2.80180000	-0.86096800
C	6.62392500	3.99893500	-0.26613000
C	5.40553400	4.06726100	0.41080800
C	4.58905000	2.94708900	0.49476500
C	-3.38856100	0.93907700	0.01357400

C	-4.69034900	1.32183000	0.01824300
C	-5.74462300	0.26364700	0.00561200
C	-5.31925100	-1.16634900	-0.01066500
C	-3.99227600	-1.45065000	-0.01433900
C	-6.39341300	-2.26520300	-0.02273900
C	-7.27541800	-2.15553100	1.24478700
C	-7.27585200	-2.12731100	-1.28722900
C	-5.77334800	-3.67486800	-0.03854400
C	-5.11129700	2.79855900	0.03576000
C	-3.89413000	3.74203400	0.04790800
C	-5.94554400	3.12374300	-1.22731500
C	-5.94736700	3.09345800	1.30504000
O	-6.93881700	0.56628800	0.00869900
H	-1.65305200	-2.99064900	-0.03266700
H	0.93024800	-3.00625500	-0.03528300
H	6.65848500	-0.14257500	1.31282800
H	8.75046700	-1.43045500	1.47476300
H	8.95452600	-3.63171500	0.34422000
H	7.02859900	-4.54352300	-0.93258800
H	4.91631100	-3.25163300	-1.07720700
H	6.51708200	0.75433200	-1.25099300
H	7.95518100	2.74591100	-1.40394900
H	7.25973000	4.87582000	-0.33414700
H	5.09114100	4.99828600	0.87138600
H	3.63540500	2.99507800	1.00664100
H	-2.61206900	1.69337400	0.02236300
H	-3.67307800	-2.48286200	-0.02630500
H	-8.01980500	-2.95775000	1.24858200
H	-6.67137400	-2.25888300	2.15142200
H	-7.79876800	-1.20279500	1.28442100

H	-8.02018500	-2.92930700	-1.30871600
H	-6.67209700	-2.21031200	-2.19614200
H	-7.79925800	-1.17395800	-1.30538800
H	-5.16067200	-3.86983200	0.84679400
H	-6.57241800	-4.42011000	-0.04656700
H	-5.16117400	-3.85010600	-0.92834200
H	-4.24185500	4.77788700	0.06021200
H	-3.26748300	3.60215900	0.93358100
H	-3.26628100	3.62369500	-0.84000800
H	-6.21789500	4.18362800	-1.22713700
H	-6.85950800	2.53504700	-1.26384900
H	-5.36910000	2.92963100	-2.13694700
H	-5.37234400	2.87738900	2.21063500
H	-6.21949000	4.15311200	1.32989900
H	-6.86150200	2.50429300	1.32607600

PTI-1 in the triplet state (OS; ub3lyp/6-311g(d))

C	-1.59094500	-0.86223500	-0.16532200
C	-1.06550500	-2.12865300	-0.37917400
C	0.33974000	-2.16486800	-0.37967200
C	0.91352500	-0.92426400	-0.16169600
S	-0.30473600	0.30782600	0.04624500
C	2.30548900	-0.60121000	-0.09290300
C	-2.99141000	-0.46933100	-0.10442200
N	3.27908600	-1.54226500	-0.26345800
C	4.41537500	-0.86795400	-0.11396600
C	4.07693300	0.55948500	0.11426100
N	2.75015300	0.66344300	0.14519900
C	5.70300700	-1.55884300	-0.12942900
C	4.92479200	1.74215700	0.23325000

C	6.79850700	-1.12697200	0.63948200
C	7.98941300	-1.84482700	0.63894300
C	8.11316300	-3.00042000	-0.13068600
C	7.02924500	-3.44645300	-0.88945900
C	5.83418500	-2.74132200	-0.88222000
C	6.17248300	1.84255600	-0.40880100
C	6.92439300	3.00819800	-0.31422800
C	6.45181600	4.09152000	0.42496100
C	5.20958400	4.00940100	1.05735000
C	4.44878400	2.85365300	0.95545800
C	-3.38155900	0.87581000	-0.30617400
C	-4.69391100	1.28254800	-0.26222800
C	-5.73433800	0.26825600	0.00545300
C	-5.32424700	-1.13569000	0.21973500
C	-3.98647600	-1.44268000	0.15775700
C	-6.38989200	-2.20134800	0.51316600
C	-7.15583700	-1.83919200	1.80939300
C	-7.38272700	-2.29206500	-0.67200700
C	-5.77099200	-3.59792400	0.71131200
C	-5.09894700	2.74548100	-0.49057200
C	-3.87858900	3.64733900	-0.75576200
C	-6.03536100	2.84788300	-1.71970300
C	-5.82320100	3.29214300	0.76441700
O	-6.93854900	0.59118300	0.05230500
H	-1.68221700	-2.99958200	-0.55936200
H	0.94028700	-3.05132800	-0.53341600
H	6.70729600	-0.24473500	1.26090000
H	8.82074400	-1.50480000	1.24786800
H	9.04563200	-3.55554400	-0.13360500
H	7.11818300	-4.34931700	-1.48494100

H	4.98259800	-3.08679300	-1.45544900
H	6.53948500	1.01786200	-1.00696200
H	7.87887700	3.07363400	-0.82627700
H	7.04338200	4.99807800	0.50150400
H	4.83390200	4.85260900	1.62785200
H	3.47768700	2.78550900	1.43023500
H	-2.60582400	1.59815300	-0.52406100
H	-3.66112900	-2.45731200	0.34078600
H	-7.89341700	-2.61633400	2.03230200
H	-6.47306400	-1.77515200	2.66209800
H	-7.67629100	-0.88921200	1.71027100
H	-8.12281700	-3.07380100	-0.47500400
H	-6.86272700	-2.55316900	-1.59878900
H	-7.90740300	-1.35123300	-0.82257000
H	-5.08237300	-3.63189600	1.56052900
H	-6.56700900	-4.31872200	0.91343300
H	-5.23875300	-3.94697100	-0.17847300
H	-4.21755900	4.67495900	-0.90813600
H	-3.17917200	3.65989500	0.08506700
H	-3.32983700	3.35265700	-1.65485300
H	-6.29742400	3.89534500	-1.89790200
H	-6.95340100	2.28458600	-1.56744100
H	-5.54079000	2.47183200	-2.62046500
H	-5.17618500	3.23563100	1.64507700
H	-6.08396700	4.34387600	0.61124600
H	-6.73620900	2.73728500	0.96889500

PTI-2 in the singlet state (CS; rb3lyp/6-311g(d))

C	0.35967600	-0.25290500	-0.00894000
C	0.81778400	-1.60227500	-0.02467200

C	2.17818100	-1.73215200	-0.02779800
C	2.86937600	-0.48930400	-0.01368000
S	1.74493000	0.85493300	0.00143700
C	4.24447800	-0.30688000	-0.00910300
C	-0.94889800	0.19689300	-0.00275200
N	5.12968500	-1.36406000	-0.01153100
C	6.31876700	-0.79401000	0.00665200
C	6.13386700	0.67727400	-0.01251500
N	4.83832800	0.93150800	-0.00192700
C	7.54371800	-1.60133700	0.08222600
C	7.11828400	1.76337000	-0.08063200
C	8.67174600	-1.17947600	0.80361900
C	9.79543100	-1.99449300	0.90031700
C	9.81629900	-3.23976300	0.27535300
C	8.69790200	-3.67326700	-0.43752000
C	7.57038000	-2.86696000	-0.52737600
C	8.33744100	1.62545700	-0.76371800
C	9.22331500	2.69459700	-0.85276100
C	8.91284800	3.91604200	-0.25820200
C	7.70040200	4.06782200	0.41581000
C	6.80837300	3.00656700	0.49755400
C	-1.40986000	1.54324800	0.01342300
C	-2.76866000	1.67686100	0.01618100
C	-3.49242200	0.44597600	0.00266900
S	-2.33754300	-0.89963300	-0.01446500
C	-4.87382100	0.25470500	0.00247700
C	-5.77321800	1.37668200	0.01553900
C	-7.12540300	1.24480800	0.01608600
C	-7.71112500	-0.12497400	0.00268300
C	-6.78440300	-1.29416000	-0.01093400

C	-5.44591900	-1.06190500	-0.01056200
C	-7.36991800	-2.71392600	-0.02475400
C	-8.23316500	-2.94058300	1.24034700
C	-8.23703500	-2.91430400	-1.29160400
C	-6.26848300	-3.79007400	-0.03760700
C	-8.06687900	2.45966100	0.03007600
C	-7.29068800	3.78975400	0.04268400
C	-8.95951300	2.45036700	-1.23459800
C	-8.95567400	2.42413300	1.29698400
O	-8.93371700	-0.29062600	0.00289800
H	0.13253900	-2.44146000	-0.03220400
H	2.72274900	-2.66637300	-0.03526000
H	8.66168300	-0.22127900	1.30900900
H	10.65476700	-1.65717600	1.47092400
H	10.69591100	-3.87138400	0.34747100
H	8.70555100	-4.64412300	-0.92272300
H	6.69325700	-3.20160500	-1.06834800
H	8.58293400	0.68716900	-1.24596600
H	10.15640400	2.57387100	-1.39363700
H	9.60811500	4.74678400	-0.32410500
H	7.45010500	5.01812200	0.87653700
H	5.85946200	3.11996200	1.00795100
H	-0.72541800	2.38287900	0.02257600
H	-3.26395700	2.63797000	0.02801300
H	-5.33957700	2.36657600	0.02509000
H	-4.76131200	-1.90109800	-0.02025900
H	-8.62644500	-3.96190200	1.24193800
H	-7.63609800	-2.81337200	2.14857600
H	-9.07239900	-2.24965800	1.27785700
H	-8.63039500	-3.93537000	-1.31319400

H	-7.64278100	-2.76828000	-2.19885100
H	-9.07635800	-2.22276600	-1.31224400
H	-5.62954100	-3.74202700	0.84917900
H	-6.73170400	-4.77973600	-0.04728000
H	-5.63213200	-3.72348400	-0.92506300
H	-7.99975800	4.62114000	0.05219900
H	-6.65990700	3.89489800	0.93060300
H	-6.66231100	3.91314400	-0.84458600
H	-9.61018400	3.33043300	-1.23607300
H	-9.58526400	1.56147300	-1.27245600
H	-8.35028300	2.48620500	-2.14299600
H	-8.34367600	2.44094300	2.20407900
H	-9.60615600	3.30406800	1.31877900
H	-9.58146800	1.53471800	1.31821900

PTI-2 in the singlet state (SB; ub3lyp/6-311g(d))

C	-0.35967600	-0.25290500	0.00894000
C	-0.81778400	-1.60227500	0.02467200
C	-2.17818100	-1.73215200	0.02779800
C	-2.86937600	-0.48930400	0.01368000
S	-1.74493000	0.85493300	-0.00143700
C	-4.24447800	-0.30688000	0.00910300
C	0.94889800	0.19689300	0.00275200
N	-5.12968500	-1.36406000	0.01153100
C	-6.31876700	-0.79401000	-0.00665200
C	-6.13386700	0.67727400	0.01251500
N	-4.83832800	0.93150800	0.00192700
C	-7.54371800	-1.60133700	-0.08222600
C	-7.11828400	1.76337000	0.08063200
C	-8.67174600	-1.17947600	-0.80361900

C	-9.79543100	-1.99449300	-0.90031700
C	-9.81629900	-3.23976300	-0.27535300
C	-8.69790200	-3.67326700	0.43752000
C	-7.57038000	-2.86696000	0.52737600
C	-8.33744100	1.62545700	0.76371800
C	-9.22331500	2.69459700	0.85276100
C	-8.91284800	3.91604200	0.25820200
C	-7.70040200	4.06782200	-0.41581000
C	-6.80837300	3.00656700	-0.49755400
C	1.40986000	1.54324800	-0.01342300
C	2.76866000	1.67686100	-0.01618100
C	3.49242200	0.44597600	-0.00266900
S	2.33754300	-0.89963300	0.01446500
C	4.87382100	0.25470500	-0.00247700
C	5.77321800	1.37668200	-0.01553900
C	7.12540300	1.24480800	-0.01608600
C	7.71112500	-0.12497400	-0.00268300
C	6.78440300	-1.29416000	0.01093400
C	5.44591900	-1.06190500	0.01056200
C	7.36991800	-2.71392600	0.02475400
C	8.23316500	-2.94058300	-1.24034700
C	8.23703500	-2.91430400	1.29160400
C	6.26848300	-3.79007400	0.03760700
C	8.06687900	2.45966100	-0.03007600
C	7.29068800	3.78975400	-0.04268400
C	8.95951300	2.45036700	1.23459800
C	8.95567400	2.42413300	-1.29698400
O	8.93371700	-0.29062600	-0.00289800
H	-0.13253900	-2.44146000	0.03220400
H	-2.72274900	-2.66637300	0.03526000

H	-8.66168300	-0.22127900	-1.30900900
H	-10.65476700	-1.65717600	-1.47092400
H	-10.69591100	-3.87138400	-0.34747100
H	-8.70555100	-4.64412300	0.92272300
H	-6.69325700	-3.20160500	1.06834800
H	-8.58293400	0.68716900	1.24596600
H	-10.15640400	2.57387100	1.39363700
H	-9.60811500	4.74678400	0.32410500
H	-7.45010500	5.01812200	-0.87653700
H	-5.85946200	3.11996200	-1.00795100
H	0.72541800	2.38287900	-0.02257600
H	3.26395700	2.63797000	-0.02801300
H	5.33957700	2.36657600	-0.02509000
H	4.76131200	-1.90109800	0.02025900
H	8.62644500	-3.96190200	-1.24193800
H	7.63609800	-2.81337200	-2.14857600
H	9.07239900	-2.24965800	-1.27785700
H	8.63039500	-3.93537000	1.31319400
H	7.64278100	-2.76828000	2.19885100
H	9.07635800	-2.22276600	1.31224400
H	5.62954100	-3.74202700	-0.84917900
H	6.73170400	-4.77973600	0.04728000
H	5.63213200	-3.72348400	0.92506300
H	7.99975800	4.62114000	-0.05219900
H	6.65990700	3.89489800	-0.93060300
H	6.66231100	3.91314400	0.84458600
H	9.61018400	3.33043300	1.23607300
H	9.58526400	1.56147300	1.27245600
H	8.35028300	2.48620500	2.14299600
H	8.34367600	2.44094300	-2.20407900

H	9.60615600	3.30406800	-1.31877900
H	9.58146800	1.53471800	-1.31821900

PTI-2 in the triplet state (TB; ub3lyp/6-311g(d))

C	-0.38752700	-0.29704500	0.16893000
C	-0.80382800	-1.62055400	0.23306900
C	-2.19691200	-1.77156000	0.20380500
C	-2.87591200	-0.56344300	0.11715300
S	-1.76093500	0.78380300	0.06171200
C	-4.28071400	-0.35423800	0.06652600
C	0.95806200	0.21654500	0.18439500
N	-5.17456000	-1.38859900	0.10349500
C	-6.36064400	-0.79838400	0.02048400
C	-6.14483800	0.66843700	-0.02799800
N	-4.83401300	0.88907300	-0.02229400
C	-7.58857500	-1.59053600	-0.06181800
C	-7.09438400	1.78019900	-0.02232000
C	-8.70651700	-1.16813000	-0.80171400
C	-9.83473300	-1.97539600	-0.90139500
C	-9.87203200	-3.21315000	-0.26174500
C	-8.76412000	-3.64876800	0.46730400
C	-7.63103400	-2.85230400	0.55930600
C	-8.34563200	1.69715600	0.61367600
C	-9.19833500	2.79530700	0.64304300
C	-8.82388300	3.99255000	0.03541000
C	-7.57957300	4.09155800	-0.58981200
C	-6.71944500	3.00257000	-0.61101200
C	1.38446000	1.52401600	0.33661200
C	2.78094000	1.67168800	0.30638300
C	3.47637600	0.48211400	0.13231300

S	2.33310900	-0.84932700	-0.00976900
C	4.90042100	0.26687800	0.06172800
C	5.79112100	1.37482100	0.05123100
C	7.15214900	1.23296800	-0.01258000
C	7.71921300	-0.13312000	-0.07195900
C	6.79283600	-1.28712000	-0.06260200
C	5.44554200	-1.04219900	0.00273200
C	7.35894000	-2.71325600	-0.12166200
C	8.16723100	-2.90458200	-1.42853200
C	8.27497800	-2.96781800	1.10054900
C	6.24586200	-3.77771100	-0.10085400
C	8.09678700	2.44423700	-0.02798400
C	7.32821800	3.77754500	0.03696600
C	9.04341000	2.38892800	1.19609700
C	8.93022300	2.44664200	-1.33287400
O	8.95009400	-0.30790400	-0.12917200
H	-0.11272300	-2.45077000	0.31360100
H	-2.72291000	-2.71573100	0.24485900
H	-8.68162900	-0.21867500	-1.32227900
H	-10.68446700	-1.63932400	-1.48675400
H	-10.75572800	-3.83864100	-0.33647400
H	-8.78509200	-4.61447500	0.96204700
H	-6.76085800	-3.18777500	1.11032700
H	-8.63905600	0.78029900	1.10969800
H	-10.15533300	2.71758000	1.14874000
H	-9.49364700	4.84623100	0.05501700
H	-7.28001300	5.02330500	-1.05872700
H	-5.74642500	3.07427300	-1.08151600
H	0.70084000	2.35107600	0.48440900
H	3.26984500	2.62886000	0.42872600

H	5.36349400	2.36682500	0.08319100
H	4.75666400	-1.87707700	0.02012300
H	8.54605800	-3.92993000	-1.48236900
H	7.53608600	-2.73736500	-2.30669600
H	9.01318600	-2.22240200	-1.47490400
H	8.65369900	-3.99420800	1.07150400
H	7.72135700	-2.84463100	2.03641300
H	9.12405500	-2.28799700	1.10831200
H	5.57085500	-3.69109300	-0.95732800
H	6.69775000	-4.77159900	-0.14647600
H	5.64826000	-3.73739000	0.81454600
H	8.04159800	4.60520300	0.02472200
H	6.66056000	3.91540000	-0.81867700
H	6.73919700	3.87391900	0.95389600
H	9.69606800	3.26746200	1.19939600
H	9.66655600	1.49765200	1.17530500
H	8.47447800	2.39439100	2.13090000
H	8.28014800	2.49288600	-2.21194900
H	9.58138700	3.32601200	-1.35473300
H	9.55141700	1.55693100	-1.40806000

PTI-3 in the singlet state (CS; rb3lyp/6-311g(d))

C	2.35093800	-0.70690900	-0.00501900
C	2.92234800	-2.00717500	-0.02008800
C	4.29248500	-2.01862200	-0.02242200
C	4.87074300	-0.72352700	-0.00831800
S	3.63249400	0.51625000	0.00612300
C	6.22703000	-0.41627600	-0.00420900
C	1.00349700	-0.36765500	-0.00054400
C	0.42878500	0.92884200	0.01482200

C	-0.94214400	0.94314500	0.01502600
C	-1.54344200	-0.34095700	0.00001800
S	-0.28255900	-1.58424400	-0.01483200
C	-2.89614100	-0.65438300	-0.00349400
C	-3.49797300	-1.93840600	-0.01758900
C	-4.86692800	-1.92438900	-0.01767800
C	-5.45114400	-0.62546100	-0.00375500
S	-4.15660600	0.58599400	0.00981700
C	-6.80601500	-0.28114600	-0.00078600
C	-7.22858700	1.08895400	0.01297300
C	-8.53424000	1.46813100	0.01560300
C	-9.58416700	0.41009200	0.00367400
C	-9.15316700	-1.01467200	-0.00986900
C	-7.82281100	-1.29555400	-0.01167700
C	-10.22241200	-2.11877800	-0.02140700
C	-11.10670900	-2.01070500	1.24454300
C	-11.10429800	-1.98667900	-1.28676000
C	-9.59755600	-3.52636700	-0.03413300
C	-8.95830600	2.94427400	0.03012000
C	-7.74446200	3.89208200	0.04178500
C	-9.79251100	3.26554100	-1.23387100
C	-9.79658500	3.23960800	1.29774400
O	-10.78216700	0.71016100	0.00481700
N	6.70374200	0.86996500	0.00262900
C	8.01894500	0.73517300	-0.01016900
C	8.33682700	-0.71064000	0.00816700
N	7.20298800	-1.38763100	-0.00822800
C	8.89801000	1.90773300	-0.08152900
C	9.62917300	-1.40469500	0.08230900
C	10.12405900	1.88319000	-0.76605700

C	10.90658800	3.02988200	-0.85805400
C	10.48461000	4.21846600	-0.26550200
C	9.26390600	4.25780000	0.40959300
C	8.47472200	3.11823200	0.49455000
C	10.71853000	-0.88108600	0.79671800
C	11.91121000	-1.59167400	0.89076000
C	12.04078200	-2.83289700	0.27080100
C	10.96209500	-3.36775400	-0.43446000
C	9.76666600	-2.66584100	-0.52209600
H	2.31416100	-2.90398600	-0.02796200
H	4.91552100	-2.90243500	-0.02948900
H	1.03696900	1.82496700	0.02521400
H	-1.53070600	1.85239300	0.02582800
H	-2.91056200	-2.84883300	-0.02736800
H	-5.46320600	-2.82638600	-0.02768000
H	-6.45589600	1.84786600	0.02135800
H	-7.50153700	-2.32752000	-0.02161900
H	-11.85056000	-2.81364200	1.24783900
H	-10.50356800	-2.11275900	2.15201500
H	-11.63016400	-1.05796000	1.28235200
H	-11.84803400	-2.78948500	-1.30680100
H	-10.49941100	-2.07133100	-2.19485800
H	-11.62779500	-1.03343100	-1.30738900
H	-8.98508900	-3.71749100	0.85228600
H	-10.39394600	-4.27463300	-0.04194400
H	-8.98344000	-3.70073800	-0.92286200
H	-8.09537100	4.92698400	0.05193500
H	-7.11833600	3.75543100	0.92853700
H	-7.11563300	3.77379000	-0.84568800
H	-10.07143500	4.32389600	-1.23470100

H	-10.70226300	2.67045600	-1.27042900
H	-9.21385400	3.07381200	-2.14271300
H	-9.22093300	3.02909900	2.20434000
H	-10.07535200	4.29778000	1.31943300
H	-10.70652700	2.64408800	1.31908300
H	10.45503200	0.97104700	-1.24740300
H	11.84622100	2.99538100	-1.40007000
H	11.09940400	5.11024400	-0.33392400
H	8.92653500	5.18160400	0.86878700
H	7.51985100	3.14378100	1.00578100
H	10.62496500	0.07426800	1.29889000
H	12.73947400	-1.17618300	1.45580200
H	12.97374500	-3.38296100	0.34099900
H	11.05419000	-4.33630200	-0.91570700
H	8.92040900	-3.07984100	-1.05726400

PTI-3 in the singlet state (SB; ub3lyp/6-311g(d))

C	2.37110500	-0.72736800	-0.00627700
C	2.92124100	-2.01704300	-0.02462600
C	4.30826300	-2.03619700	-0.02729600
C	4.88215300	-0.75727400	-0.01033100
S	3.64771200	0.48441100	0.00772100
C	6.25134100	-0.43608400	-0.00528300
C	1.00119500	-0.36052300	-0.00072000
C	0.44327900	0.91867800	0.01660100
C	-0.94992200	0.93271300	0.01683900
C	-1.53301200	-0.33470200	-0.00009900
S	-0.27886400	-1.57028900	-0.01694700
C	-2.91014700	-0.67584000	-0.00446200
C	-3.49288600	-1.94578800	-0.02007400

C	-4.88195200	-1.93379000	-0.02027300
C	-5.45342100	-0.65169200	-0.00488600
S	-4.16406400	0.55622500	0.01019100
C	-6.82787700	-0.28948200	-0.00125700
C	-7.23467500	1.07693100	0.01414800
C	-8.54361500	1.46662600	0.01752500
C	-9.59502500	0.41872500	0.00471500
C	-9.17639600	-1.00461000	-0.01079100
C	-7.84246700	-1.29476900	-0.01323400
C	-10.25018200	-2.10389400	-0.02367700
C	-11.13373500	-1.99311700	1.24271100
C	-11.13165900	-1.96539600	-1.28881600
C	-9.63222900	-3.51466000	-0.03858400
C	-8.95459900	2.94644700	0.03395400
C	-7.73292100	3.88442000	0.04608200
C	-9.78677300	3.27614600	-1.22929700
C	-9.78979000	3.24723000	1.30239900
O	-10.79628500	0.72732100	0.00689300
N	6.71045300	0.85183400	0.00873700
C	8.03092800	0.73250800	-0.00743400
C	8.36215900	-0.71134200	0.00547000
N	7.23016400	-1.39781100	-0.01547200
C	8.89368400	1.91431400	-0.08098300
C	9.65668200	-1.39654800	0.08245200
C	10.12565400	1.90252000	-0.75641400
C	10.89221500	3.05952400	-0.85049700
C	10.44866000	4.24591100	-0.26919800
C	9.22189000	4.27299200	0.39593500
C	8.44793200	3.12358800	0.48236500
C	10.74734800	-0.85988300	0.78625700

C	11.94313900	-1.56441300	0.88297100
C	12.07498700	-2.81201500	0.27621500
C	10.99523800	-3.36016400	-0.41756500
C	9.79631100	-2.66521700	-0.50710200
H	2.31025200	-2.91177500	-0.03494000
H	4.92276300	-2.92608200	-0.03672500
H	1.04826600	1.81693000	0.02842200
H	-1.53585200	1.84362300	0.02912100
H	-2.90616900	-2.85652800	-0.03093900
H	-5.47456500	-2.83845900	-0.03149700
H	-6.45806600	1.83140100	0.02328000
H	-7.52705200	-2.32843800	-0.02463100
H	-11.87998600	-2.79376900	1.24570500
H	-10.53088000	-2.09752600	2.15007400
H	-11.65389900	-1.03858900	1.28078700
H	-11.87775000	-2.76590900	-1.31073400
H	-10.52726100	-2.04962900	-2.19724800
H	-11.65195700	-1.01034400	-1.30670100
H	-9.02057200	-3.71026700	0.84730200
H	-10.43261700	-4.25862100	-0.04726600
H	-9.01928600	-3.69100400	-0.92761900
H	-8.07576600	4.92199600	0.05749700
H	-7.10752000	3.74210000	0.93237700
H	-7.10547000	3.76232900	-0.84177100
H	-10.05522400	4.33717700	-1.22943900
H	-10.70222100	2.68980100	-1.26507300
H	-9.21099700	3.07915300	-2.13882600
H	-9.21629200	3.02926800	2.20858300
H	-10.05807100	4.30803600	1.32624700
H	-10.70542300	2.66042800	1.32245300

H	10.47245000	0.99250900	-1.23040300
H	11.83602100	3.03511800	-1.38567700
H	11.05117100	5.14587300	-0.33927100
H	8.86802200	5.19528300	0.84551600
H	7.48833200	3.13896700	0.98485300
H	10.65151600	0.09978300	1.27947600
H	12.77204500	-1.13959500	1.43998400
H	13.01059700	-3.35724600	0.34843600
H	11.08945600	-4.33394200	-0.88757100
H	8.94867800	-3.08908800	-1.03202600

PTI-3 in the triplet state (TB; ub3lyp/6-311g(d))

C	-2.38274000	-0.74743700	-0.11010500
C	-2.91942200	-2.03069200	-0.06219900
C	-4.31660400	-2.05359000	-0.02100100
C	-4.88732800	-0.78416600	-0.03756800
S	-3.65519400	0.45813000	-0.09779800
C	-6.26391300	-0.45180000	-0.01059100
C	-0.99967400	-0.36354300	-0.16250300
C	-0.45398300	0.89577500	-0.33136700
C	0.95333500	0.91022900	-0.34278900
C	1.52626700	-0.33737000	-0.18244000
S	0.27826600	-1.55664700	0.00239000
C	2.91840900	-0.69534000	-0.15251700
C	3.49218600	-1.95554100	-0.19872700
C	4.89333900	-1.94291200	-0.15510000
C	5.45293700	-0.67097400	-0.07599900
S	4.16327800	0.53137300	-0.04107400
C	6.83805500	-0.29514500	-0.02282900
C	7.23296000	1.06984200	-0.01424800

C	8.54239200	1.46802800	0.03428100
C	9.59539400	0.42770500	0.08045400
C	9.18645100	-0.99576600	0.07195200
C	7.85170200	-1.29359400	0.02166900
C	10.26351100	-2.09028600	0.12170900
C	11.19558200	-1.96855700	-1.10860500
C	11.09411100	-1.95423900	1.42119600
C	9.65217900	-3.50399900	0.10501600
C	8.94329000	2.95050100	0.03969000
C	7.71668600	3.88066600	-0.01364100
C	9.72551600	3.27943600	1.33482400
C	9.82351100	3.26288000	-1.19518800
O	10.79733700	0.74321800	0.12555500
N	-6.70996400	0.83795000	-0.03281600
C	-8.03285200	0.73172200	0.02282800
C	-8.37543200	-0.71037700	0.03939600
N	-7.24542000	-1.40492500	0.04150100
C	-8.88018000	1.92163700	0.10788500
C	-9.67337800	-1.38833500	0.00157000
C	-10.09812200	1.92804700	0.80960100
C	-10.84894600	3.09423500	0.91299100
C	-10.40406600	4.27210700	0.31528000
C	-9.19099100	4.28160100	-0.37536600
C	-8.43196000	3.12337700	-0.47098100
C	-10.78295100	-0.84792200	-0.67027200
C	-11.98357200	-1.54785300	-0.73029100
C	-12.10192900	-2.79421800	-0.11801000
C	-11.00386800	-3.34647100	0.54349600
C	-9.80003000	-2.65695800	0.59575200
H	-2.30661100	-2.92407800	-0.06768400

H	-4.92587700	-2.94661500	0.01167700
H	-1.05905000	1.78485100	-0.45953300
H	1.53768500	1.81113700	-0.48436700
H	2.90786300	-2.86410900	-0.28011200
H	5.48695600	-2.84627200	-0.19601100
H	6.45354300	1.82014700	-0.05401900
H	7.54070400	-2.32862500	0.02230300
H	11.94411200	-2.76674400	-1.08686800
H	10.62928900	-2.06954100	-2.03958300
H	11.71320000	-1.01197600	-1.12042100
H	11.84212600	-2.75182800	1.46824400
H	10.45509100	-2.04564500	2.30486700
H	11.60908900	-0.99709000	1.46395100
H	9.07658500	-3.69750600	-0.80510600
H	10.45535700	-4.24410900	0.14092900
H	9.00584700	-3.68825800	0.96832300
H	8.05302500	4.92038900	-0.00678800
H	7.12598700	3.73930500	-0.92352500
H	7.05719000	3.74980200	0.84931400
H	9.98495900	4.34257100	1.35059300
H	10.64376900	2.70016000	1.40117100
H	9.11826100	3.07268700	2.22139600
H	9.28613400	3.04535500	-2.12333900
H	10.08499200	4.32559700	-1.20410900
H	10.74328800	2.68235000	-1.18329600
H	-10.44437700	1.02536000	1.29761500
H	-11.78110000	3.08414400	1.46859200
H	-10.99455800	5.17935500	0.39286700
H	-8.83615300	5.19736500	-0.83724600
H	-7.48270100	3.12481900	-0.99279500

H	-10.69782000	0.10995900	-1.16869700
H	-12.82697800	-1.12086800	-1.26328400
H	-13.04139700	-3.33580500	-0.16151400
H	-11.08802900	-4.31944700	1.01694400
H	-8.93823500	-3.08367400	1.09445500

PTI-4 in the singlet state (CS; rb3lyp/6-311g(d))

C	2.78213500	-0.93171600	-0.00780100
C	2.04727400	0.27626400	0.00322000
C	0.68189800	0.11165700	0.00186900
C	0.25502300	-1.23490200	-0.01015900
S	1.66451600	-2.30313400	-0.02019000
C	4.16612700	-1.09833900	-0.00961600
C	-1.04943400	-1.72857300	-0.01416300
C	-1.48023600	-3.07436200	-0.02517200
C	-2.84576300	-3.23558000	-0.02632400
C	-3.57595400	-2.02301800	-0.01630600
S	-2.45834600	-0.65827200	-0.00533300
C	-4.96128700	-1.86457900	-0.01477500
C	4.89732100	-2.31208800	-0.01970900
C	6.26036900	-2.14758300	-0.02001000
C	6.66638200	-0.79151600	-0.00927800
S	5.27866700	0.27801100	-0.00074200
C	7.97329200	-0.30825100	-0.00396300
C	-5.94324800	-2.88557600	-0.02283800
C	-7.23606300	-2.42811500	-0.01874900
C	-7.36748800	-1.01231500	-0.00720900
S	-5.74787300	-0.28896600	-0.00178500
C	-8.53531700	-0.24046900	-0.00052600
C	-8.48517100	1.19154900	0.01071900

C	-9.59499000	1.97815000	0.01774200
C	-10.93308200	1.32369800	0.01365400
C	-10.99281300	-0.16313900	0.00190100
C	-9.82762800	-0.86512400	-0.00459900
O	-11.96734600	2.00009600	0.02017900
C	-12.36505700	-0.85551300	-0.00243600
C	-9.51102300	3.51183500	0.02967100
C	-8.05351800	4.00926100	0.03226100
C	-10.20096700	4.08746500	-1.23103800
C	-10.19873300	4.06769600	1.30042900
C	-13.15887100	-0.46233700	1.26703200
C	-13.16110300	-0.44204500	-1.26403800
C	-12.23715000	-2.39024600	-0.01484200
N	9.06693200	-1.14260800	-0.00361400
C	10.10315900	-0.32168400	0.01285400
C	9.59869500	1.06804000	-0.01026300
N	8.27579700	1.02850700	0.00003500
C	11.47448500	-0.84122700	0.09254000
C	10.31453400	2.34647100	-0.08428500
C	12.48639500	-0.17569500	0.80300100
C	13.76112900	-0.72472600	0.90220800
C	14.05137900	-1.94337800	0.29188900
C	13.05161900	-2.61892400	-0.40901700
C	11.77539200	-2.07861000	-0.50202400
C	11.53538000	2.48291100	-0.76521200
C	12.15931500	3.72288600	-0.85923400
C	11.58138300	4.84722200	-0.27278500
C	10.36378000	4.72641200	0.39827400
C	9.73255200	3.49248400	0.48549200
H	2.53325900	1.24407600	0.01185700

H	-0.01831800	0.93825300	0.00955300
H	-0.78185600	-3.90246200	-0.03194700
H	-3.33085500	-4.20313500	-0.03413500
H	4.40975600	-3.27986200	-0.02553600
H	6.99109000	-2.94469900	-0.02322400
H	-5.68516400	-3.93706600	-0.03148000
H	-8.09231600	-3.08856800	-0.02392800
H	-7.50655400	1.65578800	0.01359400
H	-9.86210600	-1.94549800	-0.01311200
H	-8.04570800	5.10205300	0.04083700
H	-7.50168900	3.67602700	0.91624700
H	-7.50329500	3.68996500	-0.85784600
H	-10.11766000	5.17883300	-1.23378100
H	-11.25565800	3.82320400	-1.26120900
H	-9.72224900	3.71546400	-2.14212600
H	-9.71829200	3.68167500	2.20475400
H	-10.11557300	5.15890400	1.31997300
H	-11.25332800	3.80282200	1.32841700
H	-14.12566900	-0.97557100	1.27485100
H	-12.61874300	-0.75704600	2.17209300
H	-13.33892800	0.60969300	1.30520400
H	-14.12789600	-0.95514900	-1.27842100
H	-12.62255300	-0.72214300	-2.17466300
H	-13.34128900	0.63044700	-1.28468500
H	-11.71691200	-2.77131100	0.86920700
H	-13.23513800	-2.83559100	-0.01748600
H	-11.71853900	-2.75710800	-0.90582800
H	12.26922600	0.76308900	1.29811800
H	14.52793300	-0.20096000	1.46407400
H	15.04776100	-2.36724500	0.36627800

H	13.26888000	-3.57109000	-0.88276100
H	10.99029600	-2.60292500	-1.03366400
H	11.98591700	1.62101500	-1.24210000
H	13.09713400	3.81136100	-1.39833900
H	12.07264100	5.81247600	-0.34292300
H	9.90502000	5.59890500	0.85266700
H	8.78087700	3.39287600	0.99359100

PTI-4 in the singlet state (SB; ub3lyp/6-311g(d))

C	2.77031300	-0.94324800	-0.00948800
C	2.04960000	0.24514700	0.00363400
C	0.66089700	0.07024700	0.00125400
C	0.25821000	-1.25861400	-0.01368600
S	1.66447000	-2.31267500	-0.02536200
C	4.18277600	-1.12952700	-0.01114400
C	-1.06694000	-1.79276800	-0.01976600
C	-1.47269500	-3.12086800	-0.03422600
C	-2.86154500	-3.29389600	-0.03625200
C	-3.57911500	-2.10279200	-0.02339800
S	-2.47317000	-0.73848000	-0.00857000
C	-4.99641800	-1.93523700	-0.02150000
C	4.89563100	-2.33251200	-0.02145900
C	6.27675500	-2.16751200	-0.02128700
C	6.67451300	-0.82690600	-0.01027100
S	5.28546300	0.23940700	-0.00161500
C	7.99063200	-0.32210000	-0.00406100
C	-5.97042200	-2.93351300	-0.03257000
C	-7.27650000	-2.45098200	-0.02685000
C	-7.38049400	-1.05442800	-0.01110100
S	-5.75812600	-0.35693200	-0.00359600

C	-8.55154500	-0.24218300	-0.00154500
C	-8.46766100	1.17968000	0.01310100
C	-9.56633500	1.99274400	0.02288200
C	-10.91083000	1.36669000	0.01805400
C	-11.00253300	-0.11312900	0.00287700
C	-9.84663100	-0.84123800	-0.00621400
O	-11.93609100	2.06672200	0.02654300
C	-12.38670100	-0.78077500	-0.00211100
C	-9.44743800	3.52407400	0.03853900
C	-7.97906300	3.98913200	0.04168900
C	-10.12492200	4.11802600	-1.22053800
C	-10.12207100	4.09195800	1.31110500
C	-13.17236600	-0.37561000	1.26882000
C	-13.17557900	-0.34981700	-1.26253600
C	-12.28693200	-2.31772300	-0.01787500
N	9.08976600	-1.14178800	-0.00736800
C	10.11905700	-0.30752000	0.01295800
C	9.59501600	1.07729900	-0.00826400
N	8.26954900	1.01556000	0.00468800
C	11.49343900	-0.81149300	0.09849600
C	10.28800200	2.36538500	-0.08711900
C	12.50082600	-0.12625900	0.79769400
C	13.77998400	-0.66311000	0.90316400
C	14.07934500	-1.88814300	0.31007900
C	13.08436900	-2.58336900	-0.37876800
C	11.80341100	-2.05639400	-0.47702100
C	11.51282200	2.51871500	-0.75853100
C	12.11415100	3.76917300	-0.85736300
C	11.50989600	4.88711000	-0.28515600
C	10.28809200	4.74976600	0.37549300

C	9.67844600	3.50574900	0.46667300
H	2.52695500	1.21727000	0.01471600
H	-0.04120800	0.89514400	0.01039700
H	-0.77171000	-3.94673200	-0.04303000
H	-3.33803100	-4.26583600	-0.04674900
H	4.40890900	-3.30050000	-0.02783500
H	7.00289900	-2.96899900	-0.02441700
H	-5.72784900	-3.98861700	-0.04458500
H	-8.13999400	-3.10243700	-0.03414900
H	-7.48059600	1.62485500	0.01640100
H	-9.90229200	-1.92057300	-0.01718300
H	-7.94755900	5.08143800	0.05299100
H	-7.43425700	3.64192500	0.92456200
H	-7.43626600	3.66033900	-0.84942700
H	-10.01490800	5.20698700	-1.22163100
H	-11.18575100	3.87941700	-1.24957600
H	-9.65674300	3.73608500	-2.13296000
H	-9.65174100	3.69146100	2.21442100
H	-10.01217400	5.18068300	1.33429200
H	-11.18280400	3.85265200	1.33769500
H	-14.14716900	-0.87332500	1.27703400
H	-12.63634700	-0.67985600	2.17312900
H	-13.33489600	0.69918000	1.30802400
H	-14.15041000	-0.84729900	-1.27847400
H	-12.64183200	-0.63552300	-2.17420900
H	-13.33820800	0.72554200	-1.27940800
H	-11.77338000	-2.71031100	0.86490600
H	-13.29308300	-2.74423100	-0.02078600
H	-11.77589300	-2.69229300	-0.90989600
H	12.27604900	0.81687700	1.28073100

H	14.54307800	-0.12523500	1.45654300
H	15.07937600	-2.30234700	0.38920600
H	13.30932700	-3.54072700	-0.83802800
H	11.02125500	-2.59556400	-0.99775900
H	11.98273200	1.66201300	-1.22576300
H	13.05461900	3.87111200	-1.38928900
H	11.98378000	5.86069100	-0.35900300
H	9.80919800	5.61753200	0.81779800
H	8.72355200	3.39252800	0.96555300

PTI-4 in the triplet state (TB; ub3lyp/6-311g(d))

C	2.76843200	-0.93903400	-0.20318600
C	2.05871000	0.24031000	-0.34363300
C	0.66283200	0.06567600	-0.37839000
C	0.26188900	-1.25172400	-0.26399600
S	1.65868100	-2.29742900	-0.08977500
C	4.18764200	-1.13403700	-0.14265300
C	-1.07076200	-1.79582800	-0.26876100
C	-1.47742600	-3.10221700	-0.46174200
C	-2.87360300	-3.27690300	-0.41685700
C	-3.57544800	-2.10797700	-0.18410500
S	-2.46298700	-0.76462100	0.00231800
C	-4.99960000	-1.94111600	-0.08117600
C	4.89192000	-2.33573600	-0.10506300
C	6.27767400	-2.17332100	-0.05359600
C	6.67576600	-0.83773800	-0.05025500
S	5.28931500	0.23048300	-0.10818300
C	7.99425100	-0.32834800	-0.00251500
C	-5.95743400	-2.93154000	0.08549200
C	-7.26894100	-2.44662000	0.14200800

C	-7.37663900	-1.06120900	0.02876100
S	-5.76622400	-0.37075900	-0.17351300
C	-8.55242800	-0.24195300	0.05591800
C	-8.46673900	1.17632700	0.00297600
C	-9.56555300	1.99226200	0.02731400
C	-10.90680600	1.36911500	0.11167300
C	-10.99929300	-0.10836900	0.16601200
C	-9.84310200	-0.83887500	0.13711900
O	-11.93229200	2.07134600	0.13640300
C	-12.38158600	-0.77425500	0.24972100
C	-9.44535500	3.52247600	-0.02724700
C	-7.97826600	3.98398000	-0.11177700
C	-10.18028500	4.06388600	-1.27789900
C	-10.06054800	4.14520500	1.24983400
C	-13.11109000	-0.31409100	1.53544400
C	-13.22511300	-0.39667100	-0.99235900
C	-12.28135000	-2.31060400	0.29535700
N	9.09284100	-1.14482900	0.05103200
C	10.11998900	-0.30745400	0.09716000
C	9.59388800	1.07588700	0.02998000
N	8.26811000	1.00926200	-0.00667200
C	11.48961000	-0.80645800	0.24768700
C	10.28488800	2.36402800	-0.04836200
C	12.46911000	-0.10313900	0.96878600
C	13.74335500	-0.63557000	1.13630800
C	14.06585800	-1.87397400	0.58443300
C	13.09848600	-2.58713700	-0.12529400
C	11.82199900	-2.06486000	-0.28512200
C	11.53691100	2.50813500	-0.67043300
C	12.13703900	3.75884400	-0.77170600

C	11.50459000	4.88636400	-0.25094600
C	10.25600800	4.75821700	0.35982600
C	9.64754800	3.51393200	0.45273600
H	2.53970600	1.20613200	-0.43809300
H	-0.03617200	0.88265800	-0.50971200
H	-0.78282400	-3.90872600	-0.66289100
H	-3.35970300	-4.22978400	-0.58383800
H	4.40334000	-3.30256400	-0.12281100
H	7.00016800	-2.97740200	-0.01848200
H	-5.70465000	-3.97930500	0.18872400
H	-8.12497500	-3.09284600	0.28322800
H	-7.48043800	1.61949400	-0.05212400
H	-9.89852300	-1.91780800	0.16846800
H	-7.94604900	5.07568100	-0.14900200
H	-7.39326800	3.67399500	0.75910800
H	-7.47724100	3.61596200	-1.01194900
H	-10.07017700	5.15155000	-1.33019100
H	-11.24135600	3.82648400	-1.24771000
H	-9.75485700	3.64270100	-2.19396400
H	-9.54926000	3.78236000	2.14676700
H	-9.94933600	5.23365700	1.22164000
H	-11.11902000	3.90959100	1.33526700
H	-14.08343800	-0.81129100	1.60837300
H	-12.53502700	-0.57857900	2.42753800
H	-13.27393900	0.76136000	1.53498300
H	-14.19901000	-0.89386500	-0.94445700
H	-12.73129800	-0.72129000	-1.91343700
H	-13.38965500	0.67710100	-1.04780400
H	-11.72945000	-2.66564900	1.17083700
H	-13.28638400	-2.73557200	0.35466900

H	-11.80956000	-2.72357800	-0.60125200
H	12.22523600	0.85051000	1.42082200
H	14.48422900	-0.08384000	1.70595100
H	15.06227600	-2.28477200	0.71191300
H	13.34156700	-3.55489800	-0.55231200
H	11.06050000	-2.61750700	-0.82200400
H	12.02921800	1.64363000	-1.09849400
H	13.09880400	3.85349200	-1.26548900
H	11.97751000	5.86027000	-0.32645900
H	9.75545900	5.63344800	0.76151500
H	8.67253900	3.40730700	0.91254500