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Supporting Info for:

New efficient Tert-butyldiphenyl-4H-pyranylidene sensitizers for DSSC.

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TABLE OF CONTENTS

6. Differential pulse voltammograms

- **Figure S 25**: Differential pulse voltammogram of compound **9**.
- **Figure S 26**: Differential pulse voltammogram of compound **10**.
- **Figure S 27**: Differential pulse voltammogram of compound **11**.

7. UV-Visible and emission spectra

- **Figure S 28**: UV-Visible and emission spectra of compound **9**.
- **Figure S 29**: UV-Visible and emission spectra of compound **10**.
- **Figure S 30**: UV-Visible and emission spectra of compound **11**.

8. J-V curves of the optimization process

- **Figure S 31:** Photovoltaic measurements of compound **9** using 14 μm Solaronix anodes and CH_2Cl_2 as solvent for 5 different immersion times.
- **Figure S 32:** Photovoltaic measurements of compound **9** using 14 μm Solaronix anodes and acetonitrile/^{t}BuOH (1:1) as solvent for 5 different immersion times.
- **Figure S 33:** Photovoltaic measurements of compound **9** using 14 μm Solaronix anodes and THF as solvent for 5 different immersion times.
- **Figure S 34:** Photovoltaic measurements of compound **9** using 4 μm Solaronix anodes and CH_2Cl_2 as solvent for 5 different immersion times.
- **Figure S 35:** Photovoltaic measurements of compound **9** using 4 μm Dyesol anodes and CH_2Cl_2 as solvent for 5 different immersion times.
- **Figure S 36:** Photovoltaic measurements of compound **9** using 14 μm Dyesol anodes and CH_2Cl_2 as solvent for 5 different immersion times.

9. References

1. General information

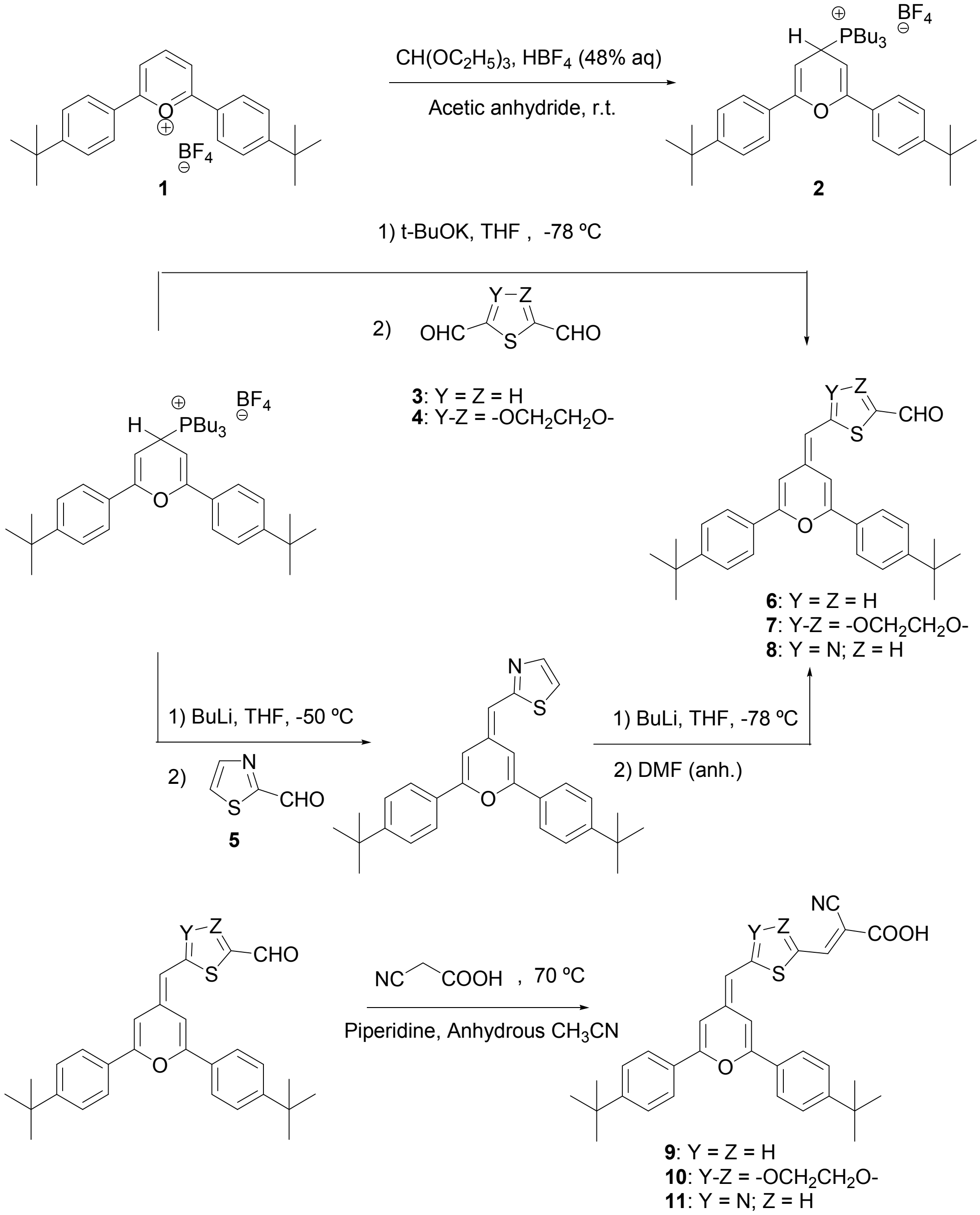
Melting points were measured at a Gallenkamp apparatus in open capillaries and are uncorrected. Infrared measurements were carried out in KBr using a Perkin-Elmer Transform Infrared 1600 spectrometer. ^{1}H and ^{13}C NMR experiments were carried out on a Bruker AV-400 or a Bruker ARX-300, at 400 or 300 MHz for ^{1}H-NMR and at 100 or 75 MHz for ^{13}C-NMR; δ values are provided using TMS as reference. As apparent resonance multiplicity, s stands for singlet, d for doublet, dd for doublet of doublets and dt for doublet of triplets. UV-Vis spectra were obtained using a UV-Vis UNICAM UV4 spectrometer. HRMS-ESI experiments took place in a Bruker μToF-Q using sodium formiate as external reference. Differential pulse voltammetries were carried out using a μ-Autolab type III potenciostate using a glassy carbon working electrode, a Pt counter electrode, a Ag/AgCl reference electrode and using Bu_4NPF_6 0.1 M as supporting electrolyte.

2. Devices fabrication and characterization

Working and counter electrodes were made of TiO_2 and platinum layers deposited onto F-doped tin oxide (FTO TCO22-15, Solaronix, with a 15 Ω/sq sheet resistance) conductive glasses. On the one hand, to obtain the anodes, the substrates were sonicated in water and soap, water and finally ethanol to clean them. Then, they were activated by an ozone treatment and then immersed in a solution of $TiCl_4$ (40 mM) at 70 ^{o}C for 30 min. Working electrodes, whose active area was 0.25 cm^2, were prepared by deposition via Screen printing of anatase pastes: Ti nanoxide T/SP and Ti nanoxide R/SP (from Solaronix) on top of it for double-layer anodes (2+2 and 12+2 microns of each paste respectively depending on the electrode) and 18NR-AO (from Dyesol) for single-layer anodes (of 4 and 14 microns). Then, they were fired using a temperature ramp, i.e., 5 min at 325˚C, 5 min at 375˚C, 5 min at 450˚C and 15 min at 500˚C. Afterwards, $TiCl_4$ process was repeated they were rinsed with ethanol and dried. They were fired 30 min at 500˚C before dye adsorption in 0.1 mM dye solutions. On the other hand, counter electrodes were produced by spreading a platinum precursor onto thermally activated FTO substrates with small holes that allowed electrolyte introduction later on. Then, thermal decomposition of this precursor gave platinum particles on the surface, which were fired 15 min at 450˚C before using them. Both electrodes were assembled by means of layer of Surlyn (Meltonix 1170-60 from Solaronix) that melts at 120˚C. As electrolyte, a mixture of 1-butyl-3-methylimidazolium iodide (0.53 M), LiI (0.10 M), I_2 (0.050 M), tert-butylpyridine (0.52 M) in acetonitrile was used (LP1 electrolyte).

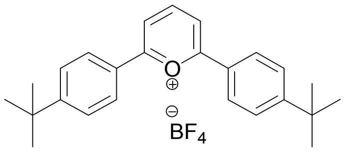
Photovoltaic measurements of the devices were carried out using a solar simulator model 10500 (Abet Technologies) as irradiating source, whose illumination intensity was 100 mW/m^2 using a ReRa silicon reference cell equipped with a 150 W xenon lamp. A Keithley 2401 SourceMeter was used to measure the applied potential and the obtained current. IPCE (Incident photon-to-current efficiency) experiments were carried out using a homemade set up using a 150 W xenon lamp, a monochromator and a Keithley 2401 SourceMeter. Impedance spectroscopy measurements were carried out using a μ-Autolab type III potenciostate equipped with a FRA module measuring between 0.1 and 100000 Hz.

3. Synthetic details



Scheme 1: Synthetic route of the dyes **9**-**11**.

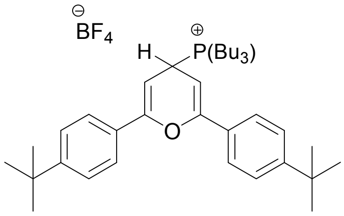
4’-tert-butyl-2,6-diphenylpyrylium tetrafluoroborate (1)



A solution of triethyl orthoformate (5 mL, 30 mmol) and 4-*tert*-butylacetophenone (1.76 g, 9.99 mmol) at room temperature was prepared. Then, a mixture composed by HBF_4 (0.5 mL, 48% in water) and acetic anhydride at 0 ^oC was added dropwise. The solution was stirred for 90 min at room temperature and then at 50 ^oC for 30 min. After that, the solution was cooled down to room temperature, added dropwise over diethyl ether at 0 ^oC (250 mL) and left overnight. The orange solid that precipitated was filtered and kept in a solution of acetone (15 mL) and 2 drops of HBF_4 (0.5 mL, 48% in water) at reflux for one hour. Then, the solid precipitated by adding diethyl ether at 0 ^oC. Yield: yellow solid (898 mg, 42%).

Mp 233–235 ^oC. IR (KBr): cm^{-1} 3106 (Csp^2-H), 2965 (Csp^3-H), 1605 (C=C). ^{1}H NMR (300 MHz, Acetone-d6): δ (ppm) 9.17 (t, J = 8.3 Hz, 1H), 8.82 (d, J = 8.3 Hz, 2H), 8.48 (dt, J_1 = 8.9 Hz, J_2 = 2.1 Hz, 4H), 7.88 (dt, J_1 = 8.9 Hz, J_2 = 2.1 Hz, 4H), 1.42 (s, 18H). ^{13}C NMR (75 MHz, Acetone-d6): δ (ppm) 173.8, 161.7, 158.8, 130.7, 129.1, 128.2, 120.7, 37.1, 32.1. HRMS (ESI$^+$): *m/z* calcd for $[C_{25}H_{29}O]^+$: 345.2213, found: 345.2200.

Tributyl(2,6-bis(4- tert -butylphenyl)-4H-pyran-4-yl)phosphonium tetrafluoroborate (2)

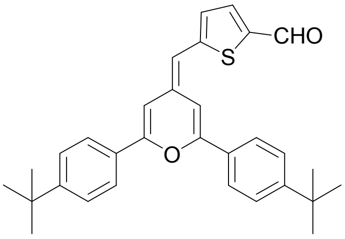


A solution of 4’-*tert*-butyl-2,6-diphenylpyrylium tetrafluoroborate **1** (523 mg, 1.21 mmol) in anhydrous acetonitrile (3.5 mL) was purged with argon. Then, tributylphosphine was added (310 μL, 1.24 mmol) and the mixture was stirred for 2 h at room temperature. To precipitate the salt, diethyl ether at 0 ^oC (100 mL) was added and then the solid was washed with cold diethyl ether. Yield: white solid (516 mg, 68%)

Mp 185–187 ^oC. IR (KBr): cm^{-1} 2961 (Csp^3-H), 1687 (C=C). ^{1}H NMR (400 MHz, Acetone-d6): δ (ppm) 7.78 (dt, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 4H), 7.54 (dt, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 4H), 5.80 (dd, J_1 = 5.0 Hz, J_2 = 2.8 Hz, 2H), 4.69 (dt, J_1 = 13.6 Hz, J_2 = 5.0 Hz, 1H), 2.59 (m, 6H), 1.82 (m, 6H), 1.52 (m, 6H), 1.35 (s, 18H), 0.93 (t, J = 7.4 Hz, 9H). ^{13}C NMR (75 MHz, Acetone-d6): δ (ppm) 154.8, 131.9, 127.4, 126.7, 126.7, 90.9, 90.8, 36.3, 32.3 (d, $J_{C\text{-}P}$ = 19.7 Hz), 25.7 (d, $J_{C\text{-}P}$ = 14.8 Hz), 25.3

(d, $J_{C\text{-}P}$ = 5.0 Hz), 18.5 (d, $J_{C\text{-}P}$ = 44.1 Hz), 14.6. MS (MALDI$^+$): *m/z* calcd for $[C_{37}H_{55}OP]^+$: 546.4, found: 546.4.

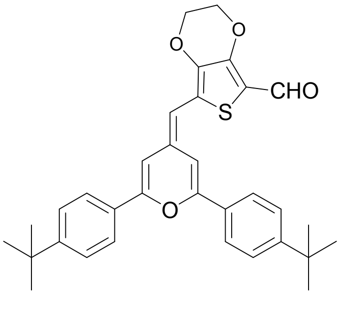
5-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)thiophene-2-carbaldehyde (6)



A solution of tributyl(2,6-bis(4-*tert*-butylphenyl)-4*H*-pyran-4yl)phosphonium tetrafluoroborate **2** (234 mg, 0.37 mmol) and potassium *tert*-butoxide (49 mg, 0.44 mmol) in anhydrous THF (15 mL) was prepared, cooled down to –78ºC and stirred for 15 min. Then, thiophene-2,5-dicarbaldehyde **3** (61 mg , 0.44 mmol) in anhydrous THF (5 mL) was added dropwise. Reaction was warmed to room temperature overnight and then it was quenched with NH_4Cl. The organic layer was extracted with ethyl acetate and dried over anhydrous $MgSO_4$. Afterwards, the solvent was removed and the solid was purified by silica gel column chromatography (hexane/ethyl acetate 8:2). Yield: red solid (86 mg, 50%).

Mp 148–150 ºC. IR (KBr): cm^{-1} 2960 (Csp^3-H), 1644 (C=O), 1567 (C=C). ^{1}H NMR (300 MHz, THF-d^8): δ (ppm) 9.78 (s, 1H), 7.82 (d, *J* = 8.6 Hz, 2H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.67 (d, *J* = 4.0 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 7.20 (d, *J* = 1.6 Hz, 1H), 7.01 (d, *J* = 4.0 Hz, 1H), 6.64 (d, *J* = 1.6 Hz, 1H), 6.17 (s, 1H), 1.37 (s, 9H), 1.35 (s, 9H). ^{13}C NMR (75 MHz, THF-d8): δ (ppm) 181.9, 156.2, 154.4, 153.8, 153.5, 152.7, 141.0, 137.7, 133.5, 131.2, 131.1, 127.0, 126.8, 126.6, 126.1, 125.5, 109.0, 107.7, 103.0, 35.7, 35.6, 31.7 (6C). HRMS (ESI$^+$): *m/z* calcd for $[C_{31}H_{33}O_2S]^+$ $[M+H]^+$: 469.2196, found: 469.2200.

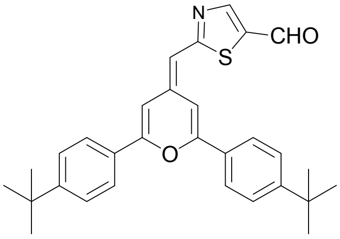
7-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)-2,3-dihydrothieno[3,4-b][1,4]dioxine-5-carbaldehyde (7)



A solution of tributyl(2,6-bis(4-*tert*-butylphenyl)-4*H*-pyran-4yl)phosphonium tetrafluoroborate **2** (411 mg, 0.65 mmol) and potassium *tert*-butoxide (86 mg, 0.77 mmol) in anhydrous THF (15 mL) was prepared, cooled down to –80ºC and stirred for 15 min. Then, 2,3-dihydrothieno[3,4-b][1,4]dioxine-5,7-dicarbaldehyde **4**[1] (61 mg , 0.44 mmol) in anhydrous THF (5 mL) was added dropwise. Reaction was warmed to room temperature overnight and then it was quenched with NH_4Cl. The organic layer was extracted with ethyl acetate and dried over anhydrous $MgSO_4$. Afterwards, the solvent was removed and the solid was purified by silica gel column chromatography (hexane/ethyl acetate 7:3). Yield: red solid (166 mg, 48%).

Mp 153–155 ºC. IR (KBr): cm^{-1} 2959 (Csp^3-H), 1629 (C=O), 1476 (C=C). ^1H NMR (400 MHz, CD_2Cl_2): δ (ppm) 9.80 (s, 1H), 7.76 (d, J = 8.2 Hz, 2H), 7.64 (d, J = 8.2 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.06 (s, 1H), 6.42 (s, 1H), 6.00 (s, 1H), 4.29 (m, 4H), 1.39 (s, 9H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ (ppm) 178.3, 155.4, 154.1, 153.5, 153.0, 149.2, 137.4, 132.7, 130.4, 130.3, 129.8, 126.3, 126.2, 125.6, 125.0, 113.7, 108.8, 103.3, 102.4, 66.1, 65.2, 35.3, 35.3, 31.5 (6C). HRMS (ESI$^+$): *m/z* calcd for $[C_{33}H_{35}O_4S]^+$ $[M+H]^+$: 527.2251, found: 527.2235.

2-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)thiazole-5-carbaldehyde (8)

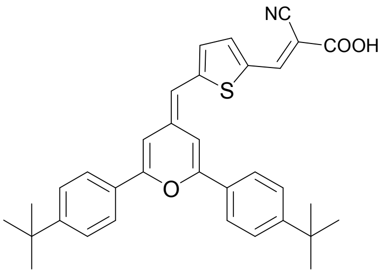


A solution of tributyl(2,6-bis(4-*tert*-butylphenyl)-4*H*-pyran-4yl)phosphonium tetrafluoroborate **2** (368 mg, 0.58 mmol) in anhydrous THF (5 mL) was prepared, purged with argon and cooled down to –78ºC. Then, *n*-BuLi (1.6 M in hexanes) (0.36 mL, 0.58 mmol) was added dropwise and the mixture was stirred for 15 min. To this solution, thiazole-2-carbaldehyde **5** (55 mg, 0.49 mmol) in anhydrous THF (5 mL) was added dropwise and the mixture was warmed to 0ºC for 4 h. Saturated NH_4Cl solution was added to quench the reaction and the solvent was evaporated. The organic layer was extracted with ethyl acetate and dried over anhydrous $MgSO_4$. Then, the product was purified by silica gel column chromatography (hexane/ethyl acetate 8:2). The resulting solid was dissolved in anhydrous THF (15 mL), purged with argon and cooled down to –45 ºC. Then, *n*-BuLi (1.6 M in hexanes) (0.44 mL, 0.71 mmol) was added and the mixture was stirred for 15 min. To this solution, anhydrous DMF (103 µL, 1.3 mmol) was added dropwise and the mixture was warmed to room temperature overnight. The reaction was quenched by adding saturated NH_4Cl solution. The organic layer was extracted with ethyl acetate and dried over anhydrous $MgSO_4$. Afterwards, the solvent was removed and the solid was purified by silica gel column chromatography (hexane/ethyl acetate 9:1). Yield: red solid (103 mg, 49%).

Mp 108–110 ºC. IR (KBr): cm^{-1} 2961 (Csp^3-H), 1650 (C=O), 1548 (C=C). ^1H NMR (400 MHz, CD_2Cl_2): δ (ppm) 9.92 (s, 1H), 8.44 (d, J = 1.8 Hz, 1H), 8.32 (s, 1H), 7.88 (d, J = 8.5 Hz, 2H), 7.79

(d, *J* = 8.5 Hz, 2H), 7.54 (m, 4H), 6.62 (d, *J* = 1.8 Hz, 1H), 6.10 (s, 1H), 1.38 (s, 9H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ (ppm) 181.9, 175.0, 157.2, 155.8, 154.6, 154.4, 154.3, 139.5, 135.2, 130.3, 130.0, 126.4, 126.4, 125.9, 125.4, 107.9, 104.7, 104.1, 35.4, 35.4, 31.5 (6C). HRMS (ESI$^+$): *m/z* calcd for $[C_{30}H_{32}NO_2S]^+$ $[M+H]^+$: 470.2148, found: 470.2135.

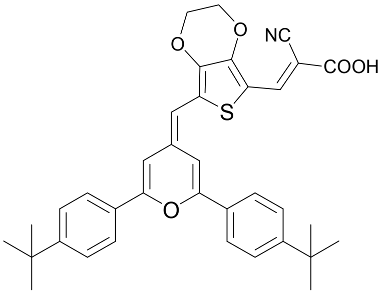
(2E)-3-(5-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)thiophen-2-yl)-2-cyanoacrylic acid (9)



To a solution of 5-((2,6-bis(4-tert-butylphenyl)-4*H*-pyran-4-ylidene)methyl)thiophene-2-carbaldehyde **6** (122 mg, 0.26 mmol) and 2-cyanoacetic acid (35 mg, 0.41 mmol) in anhydrous acetonitrile (19 mL), piperidine (150 µL, 1.4 mmol) was added. The mixture was refluxed for 3 days under argon atmosphere and then cooled down to room temperature. Final compound was precipitated by adding HCl (5mL, 1M) and was sequentially washed with hexane, hexane/CH_2Cl_2 (9:1) and hexane/CH_2Cl_2 (8:2). Yield: dark violet solid (102 mg, 73%).

Mp 208–210 °C. IR (KBr): cm^{-1} 2961 (Csp^3-H), 2211 (C≡N), 1650 (C=C). ^{1}H NMR (400 MHz, THF-d8): δ (ppm) 8.28 (s, 1H), 7.91 (d, *J* = 8.5 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 4.2 Hz, 1H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 7.44 (d, *J* = 1.6 Hz, 1H), 7.06 (d, *J* = 4.2 Hz, 1H), 6.76 (d, *J* = 1.6 Hz, 1H), 6.28 (s, 1H), 1.37 (s, 9H), 1.36 (s, 9H). ^{13}C NMR (75 MHz, THF-d8): δ (ppm) 164.8, 156.6, 154.5, 154.1, 153.9, 153.9, 146.0, 139.6, 134.4, 133.5, 130.8, 127.2, 126.8, 126.6, 126.1, 125.6, 177.9, 109.2, 107.9, 103.3, 96.3, 35.7, 35.6, 31.6 (6C). HRMS (ESI$^+$): *m/z* calcd for $[C_{34}H_{34}NO_3S]^+$ $[M+H]^+$: 536.2254, found: 536.2243.

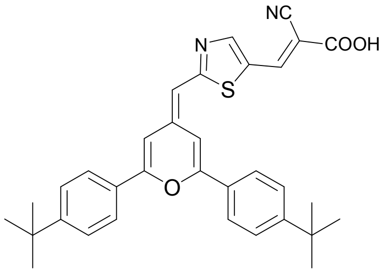
(2E)-3-(5-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)-2,3-dihydrothieno[3,4-b][1,4]dioxin-7-yl)-2-cyanoacrylic acid (10)



To a solution of 7-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)-2,3-dihydrothieno[3,4-b][1,4]dioxine-5-carbaldehyde **7** (116 mg, 0.22 mmol) and 2-cyanoacetic acid (37 mg, 0.44 mmol) in anhydrous acetonitrile (20 mL), piperidine (160 µL, 1.5 mmol) was added. The mixture was refluxed for 1 day under argon atmosphere and then cooled down to room temperature. Final compound was precipitated by adding HCl (5mL, 1M) and was sequentially washed with distilled water, hexane and hexane/CH_2Cl_2 (9:1). Yield: dark violet solid (109 mg, 83%).

Mp 180–182 ^{o}C. IR (KBr): cm^{-1} 2962 (Csp^3-H), 2204 (C≡N), 1651 (C=O), 1538 (C=C). ^{1}H NMR (300 MHz, THF-d8): δ (ppm) 8.25 (s, 1H), 7.90 (d, *J* = 8.5 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.54 (t, *J* = 8.0 Hz, 4H), 7.40 (d, *J* = 1.6 Hz, 1H), 6.80 (d, *J* = 1.6 Hz, 1H), 6.19 (s, 1H), 4.40 (m, 2H), 4.34 (m, 2H), 1.37 (s, 9H), 1.36 (s, 9H). ^{13}C NMR (75 MHz, THF-d8): δ (ppm) 165.4, 156.34, 154.5, 154.1, 153.9, 149.0, 140.2, 138.1, 133.8, 131.1, 130.9, 130.8, 126.8, 126.6, 126.0, 125.6, 118.7, 109.8, 109.5, 103.9, 103.4, 91.8, 67.0, 65.8, 35.7, 35.6, 31.7 (6C). HRMS (ESI$^+$): *m/z* calcd for $[C_{36}H_{35}NO_5S]^+$: 593.2230, found: 593.2202.

(2E)-3-(2-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)thiazol-5-yl)-2-cyanoacrylic acid (11)



To a solution of 2-((2,6-bis(4-tert-butylphenyl)-4H-pyran-4-ylidene)methyl)thiazole-5-carbaldehyde **8** (98 mg, 0.21 mmol) and 2-cyanoacetic acid (36 mg, 0.42 mmol) in anhydrous acetonitrile (15 mL), piperidine (118 µL, 1.1 mmol) was added. The mixture was refluxed for 3 days under argon atmosphere and then cooled down to room temperature. Final compound was precipitated by adding HCl (5mL, 1M) and was washed with distilled water and hexane. Yield: dark violet solid (89 mg, 79%).

Mp 198−200 ^{o}C. IR (KBr): cm^{-1} 2961 (Csp^3-H), 2219 (C≡N), 1648 (C=O), 1531 (C=C). ^{1}H NMR (500 MHz, THF-d8): δ (ppm) 8.61 (s, 1H), 8.39 (s, 1H), 8.33 (s, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H) , 6.86 (s, 1H), 6.24 (s, 1H), 1.38 (s, 9H), 1.37 (s, 9H). ^{13}C NMR (125 MHz, THF-d8): δ (ppm) 175.3, 164.5, 157.6, 156.7, 156.3, 154.7, 154.5, 144.9, 140.1, 131.1, 130.8, 128.8, 126.9, 126.8, 126.4, 126.0, 117.1, 108.7, 105.8, 104.7, 99.5, 35.7, 35.7, 31.6 (6C). HRMS (ESI$^+$): *m/z* calcd for $[C_{33}H_{32}N_2NaO_3S]^+$ $[M+Na]^+$: 559.2026, found: 559.2002.

4. NMR Spectra

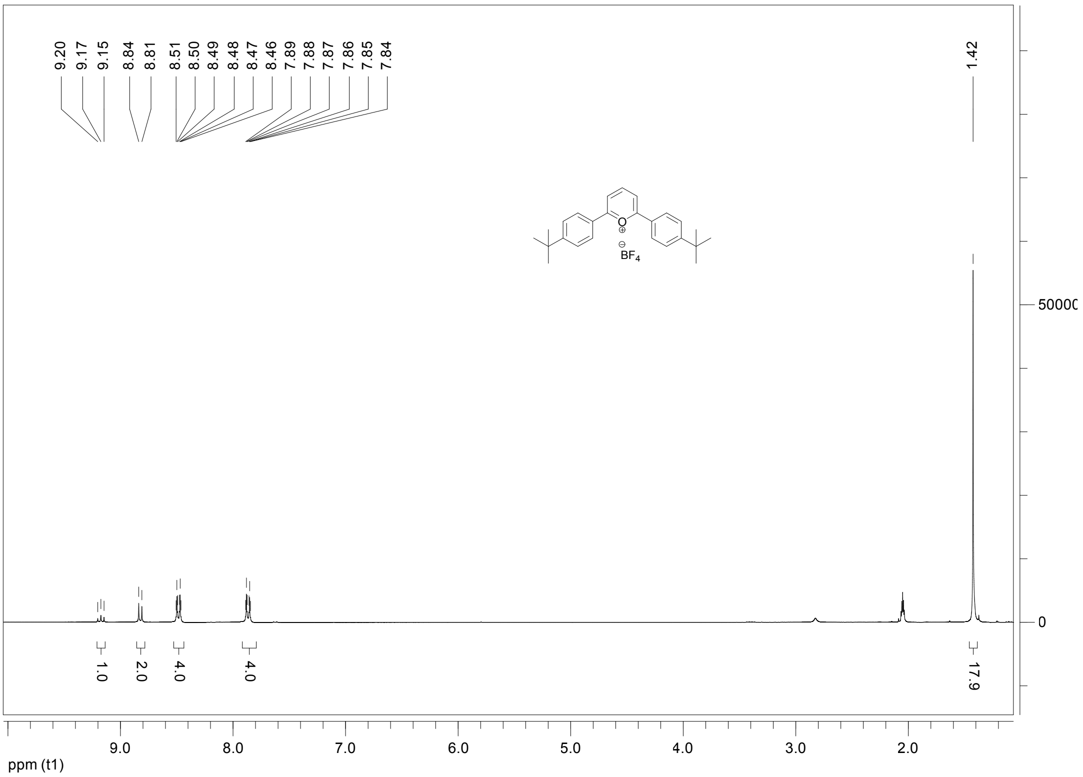


Figure S 1. *^{1}H-NMR spectrum of compound* ***1****.*

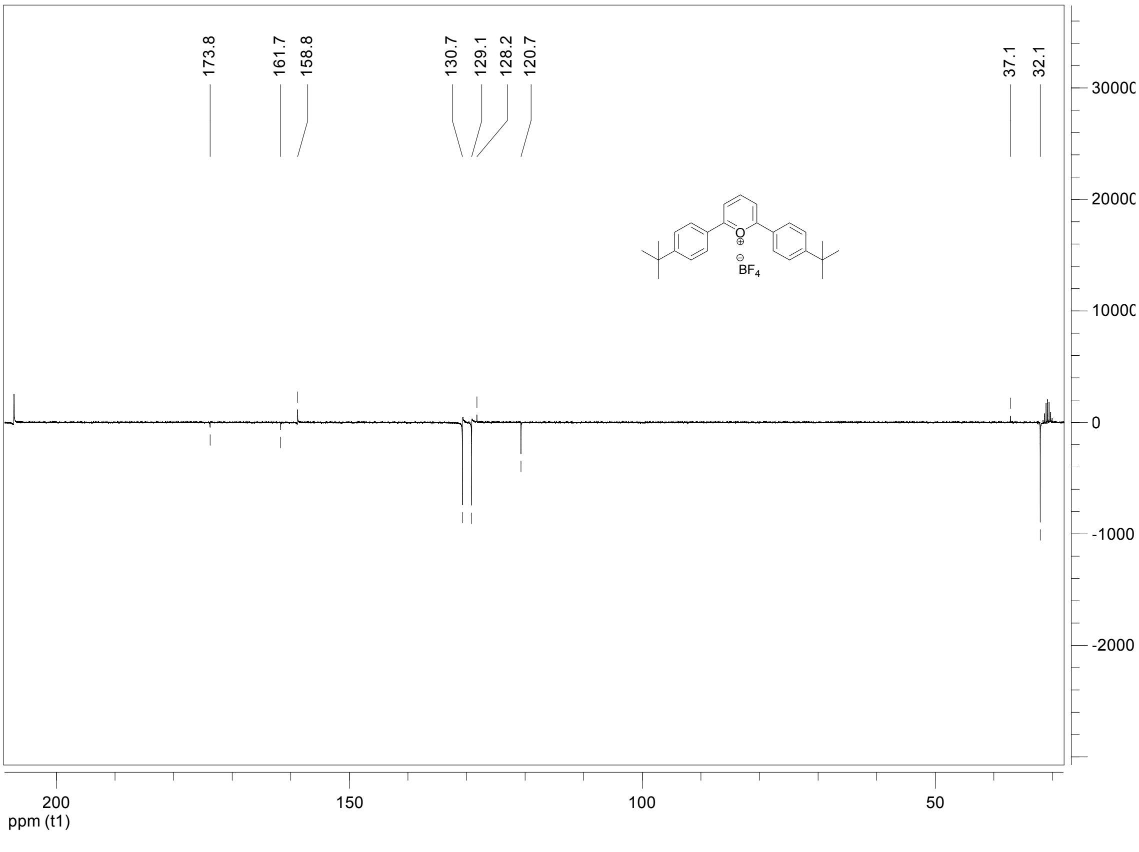


Figure S 2. *^{13}C-NMR spectrum of compound* ***1****.*

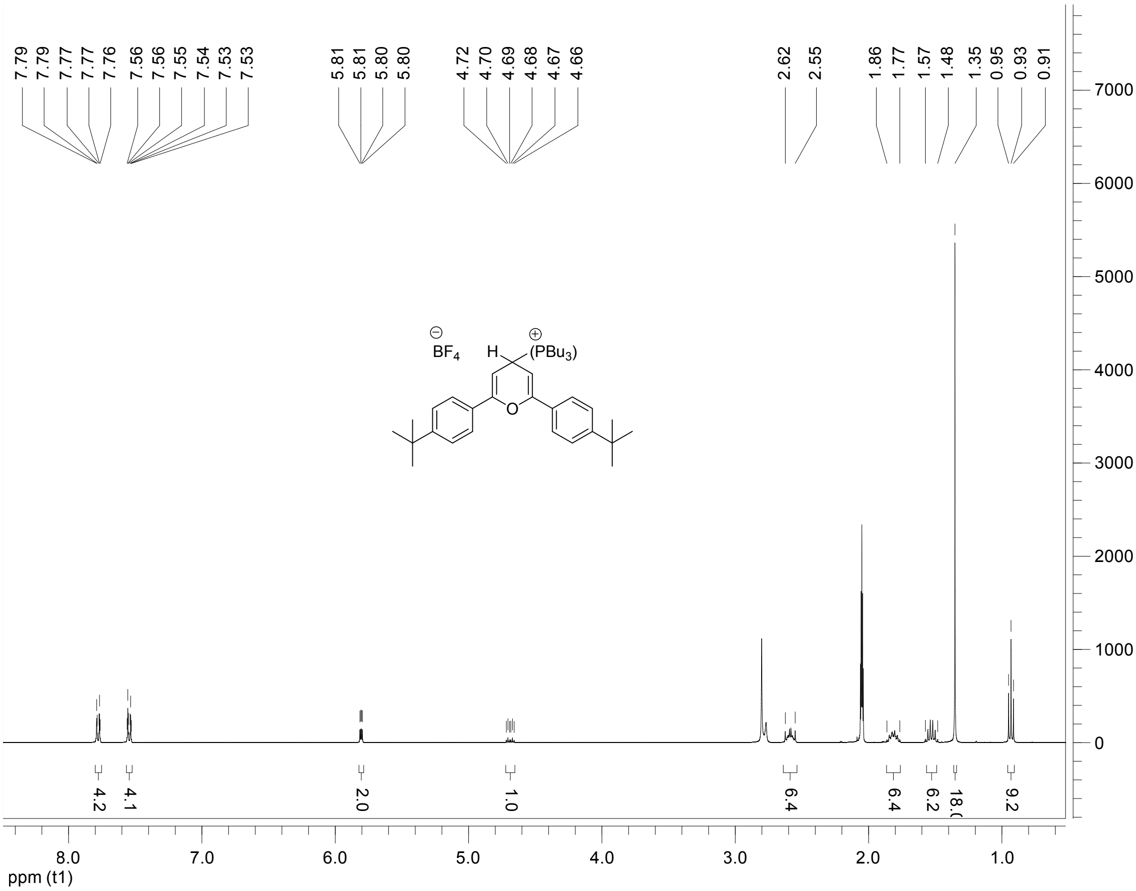


Figure S 3. *^{1}H-NMR spectrum of compound* ***2.***

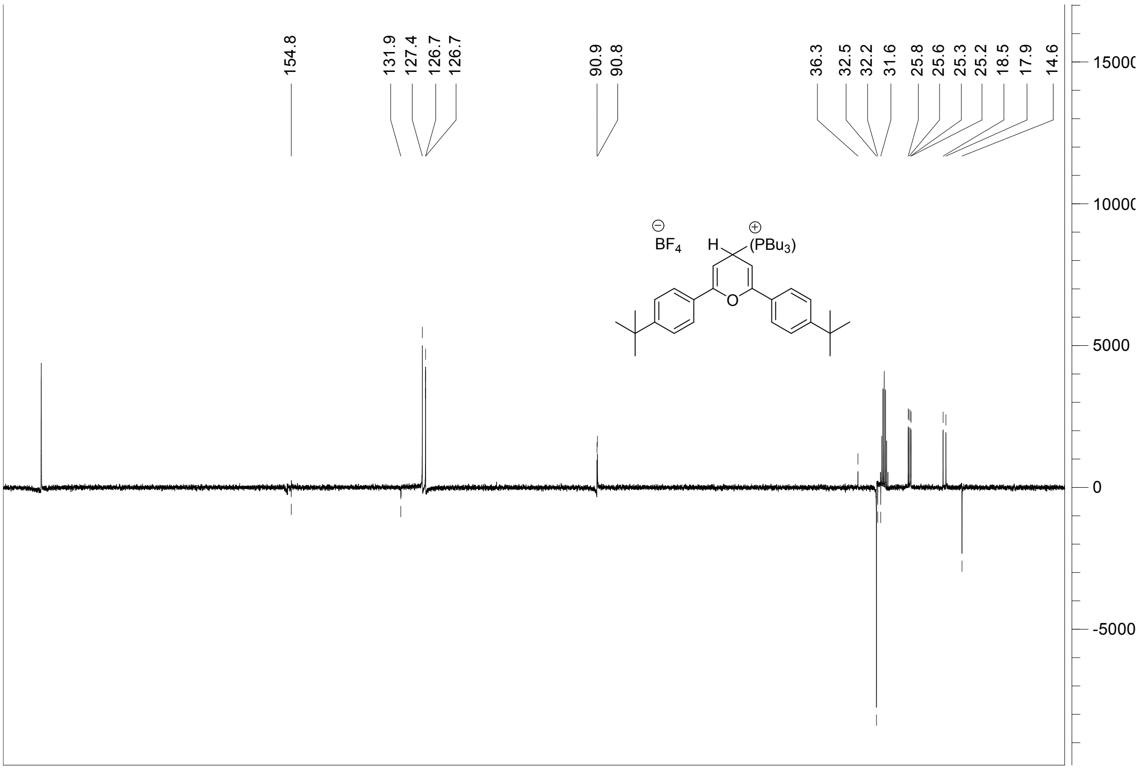


Figure S 4. *^{13}C-NMR spectrum of compound* ***2.***

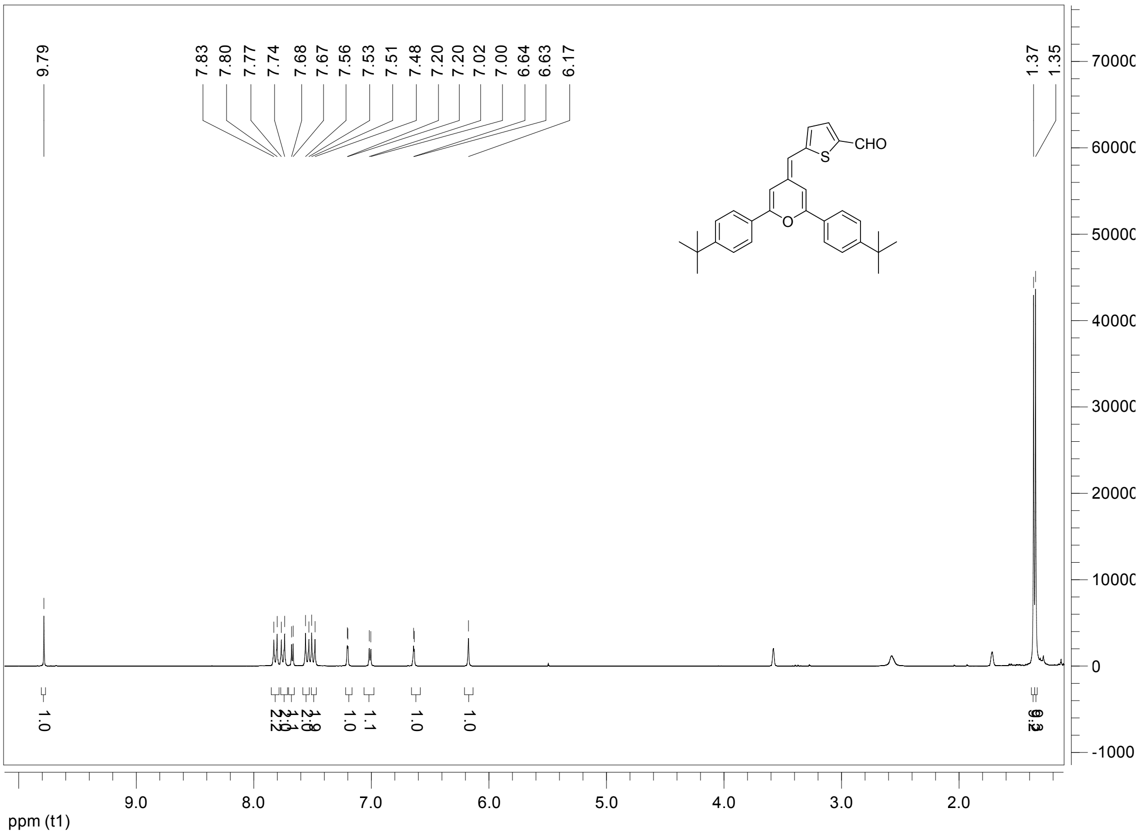


Figure S 5. *^{1}H-NMR spectrum of compound **6**.*

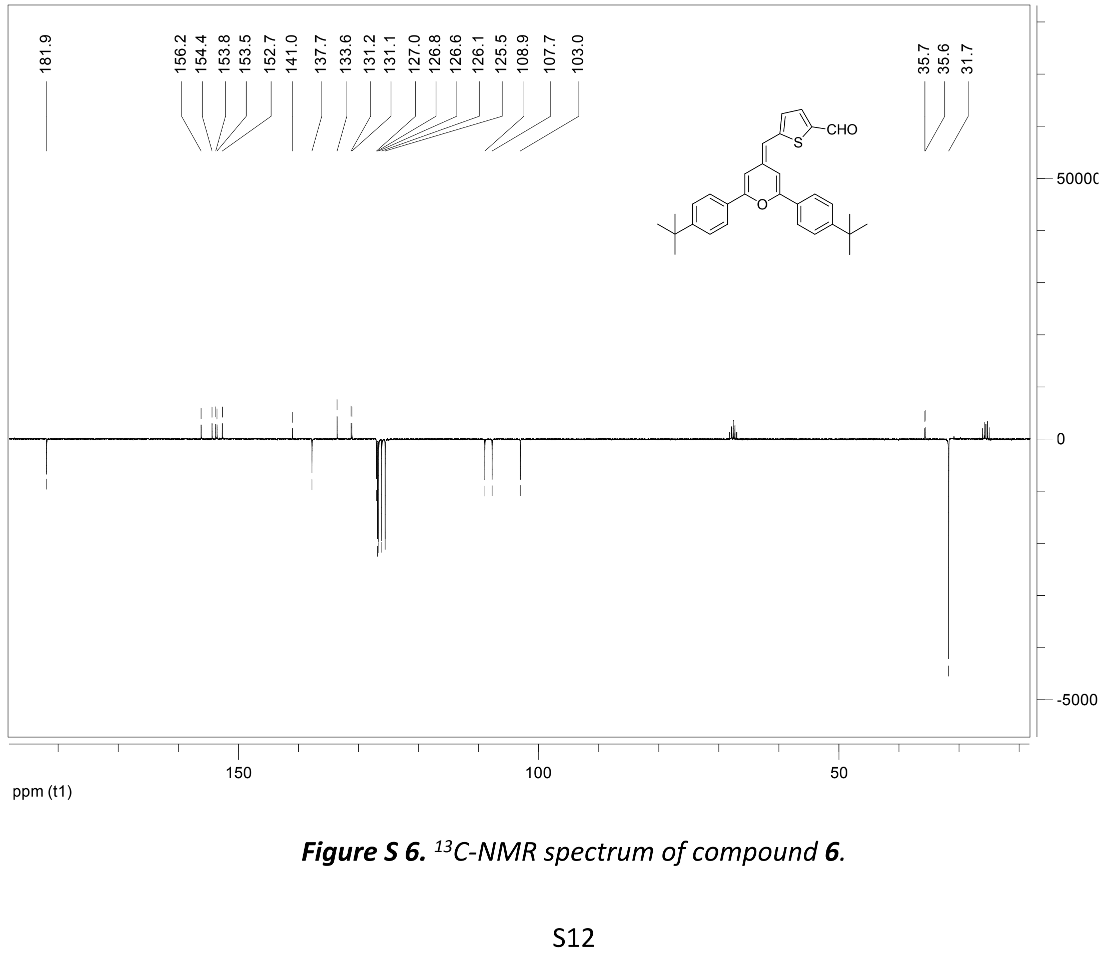


Figure S 6. *^{13}C-NMR spectrum of compound **6**.*

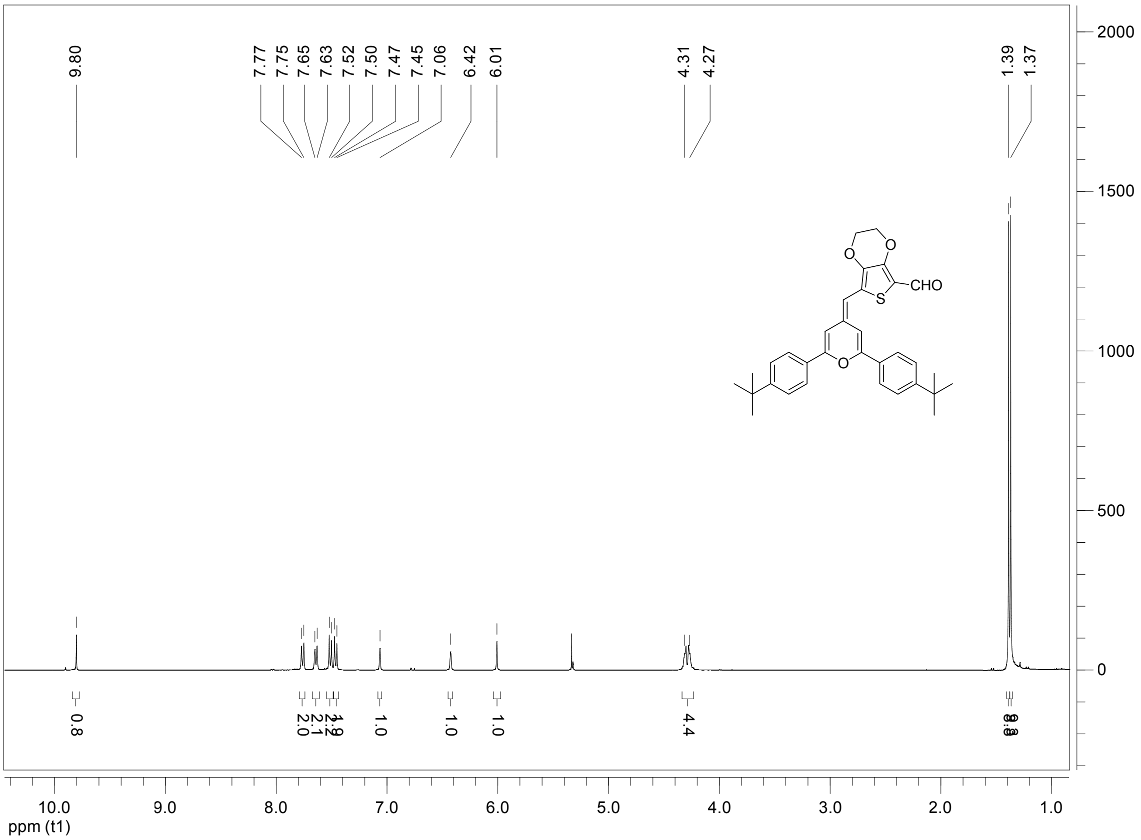


Figure S 7. ^{1}H-NMR spectrum of compound **7**.

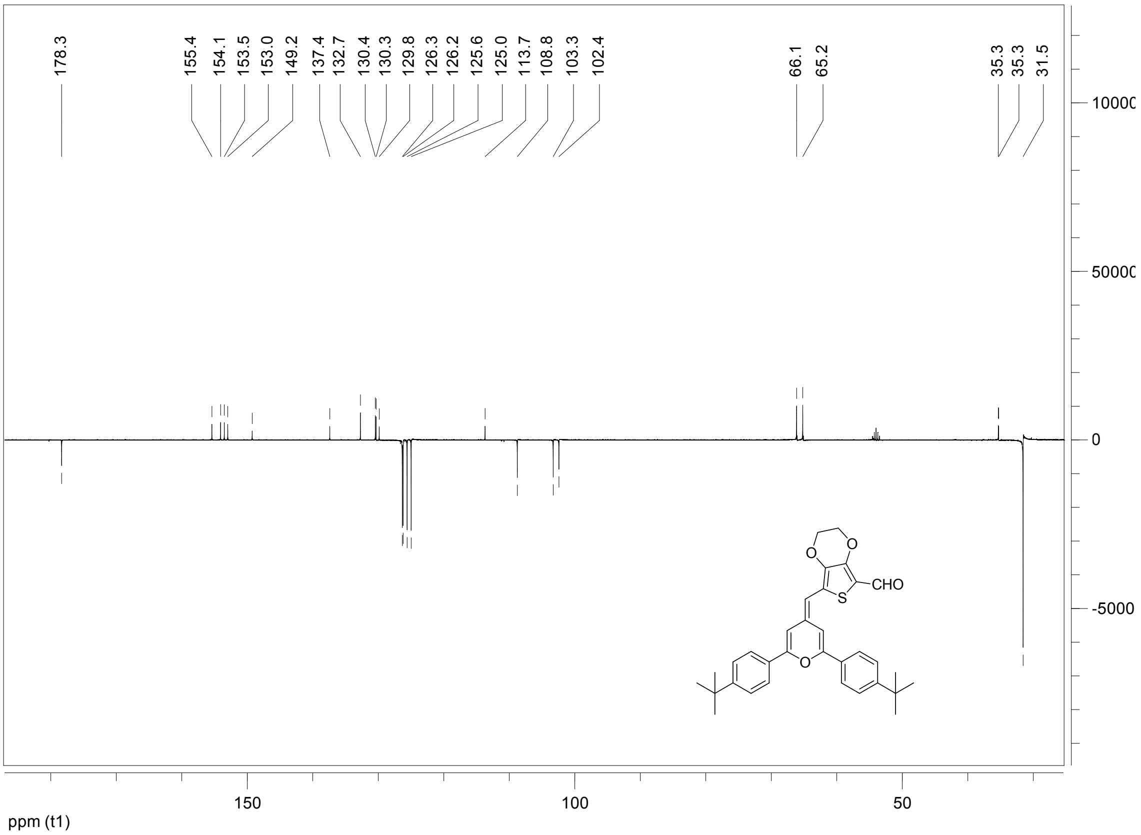


Figure S 8. ^{13}C-NMR spectrum of compound **7**.

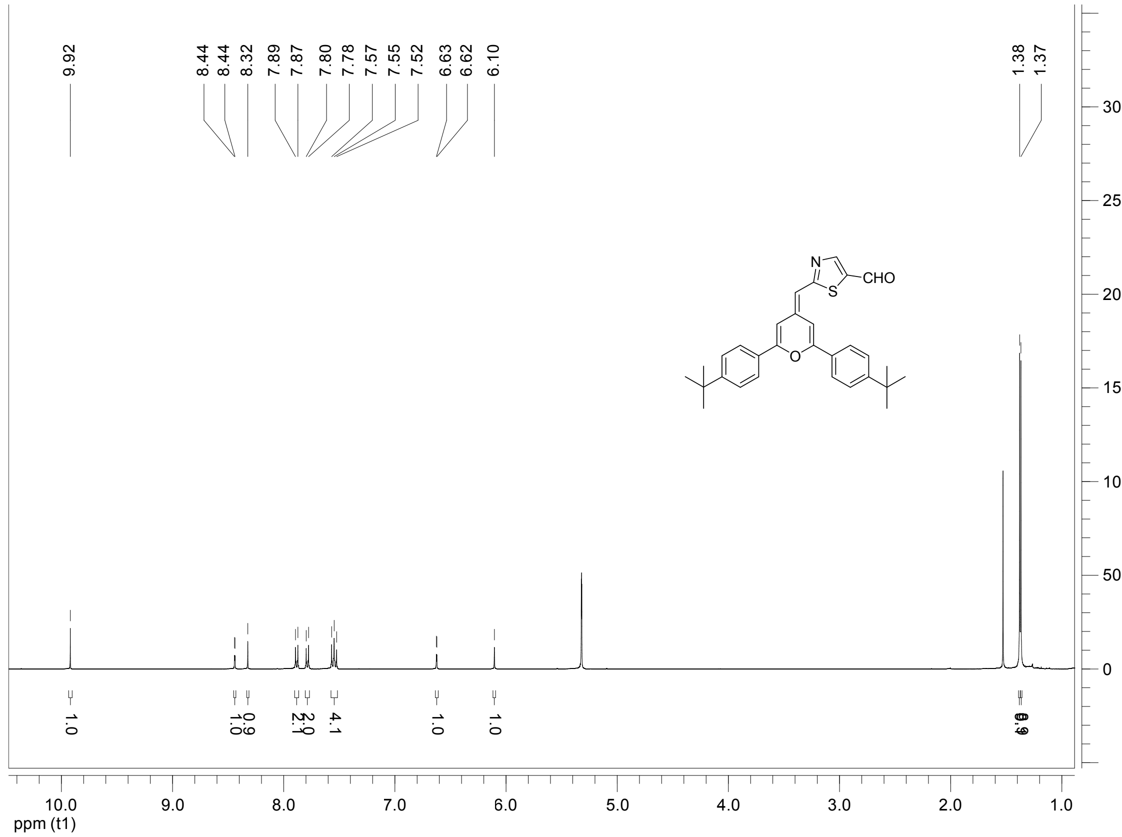


Figure S 9. *^{1}H-NMR spectrum of compound **8**.*

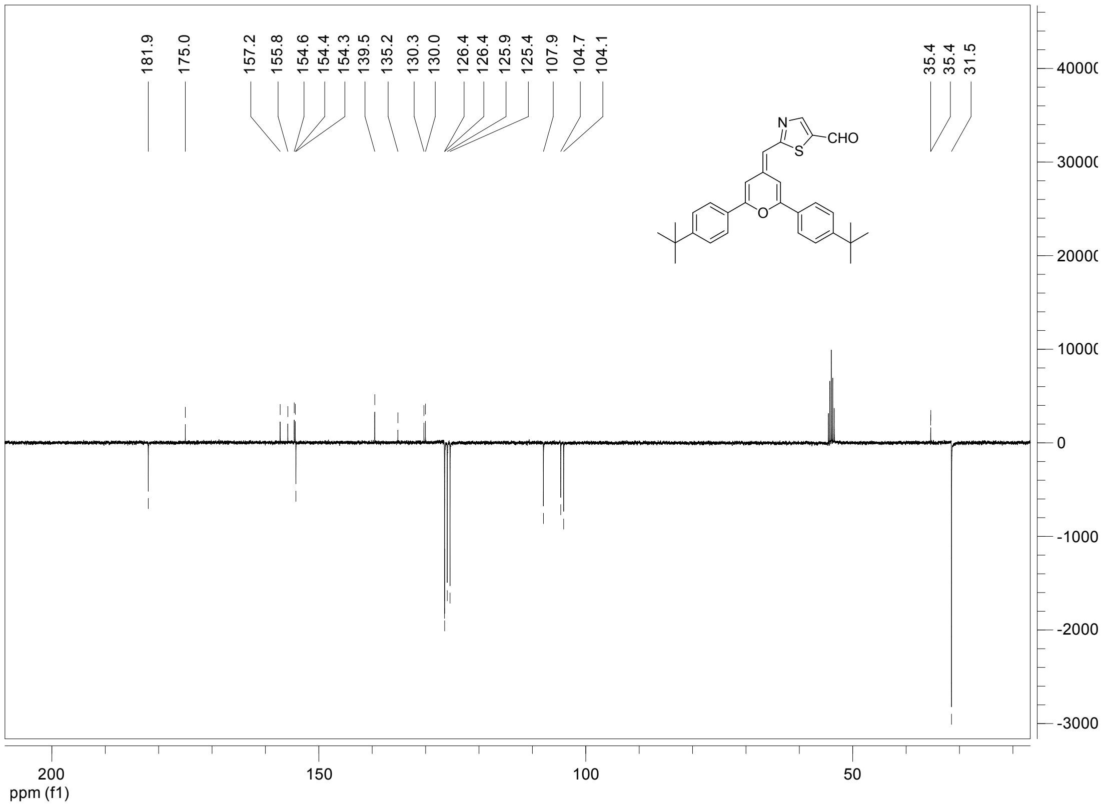


Figure S 10. *^{13}C-NMR spectrum of compound **8**.*

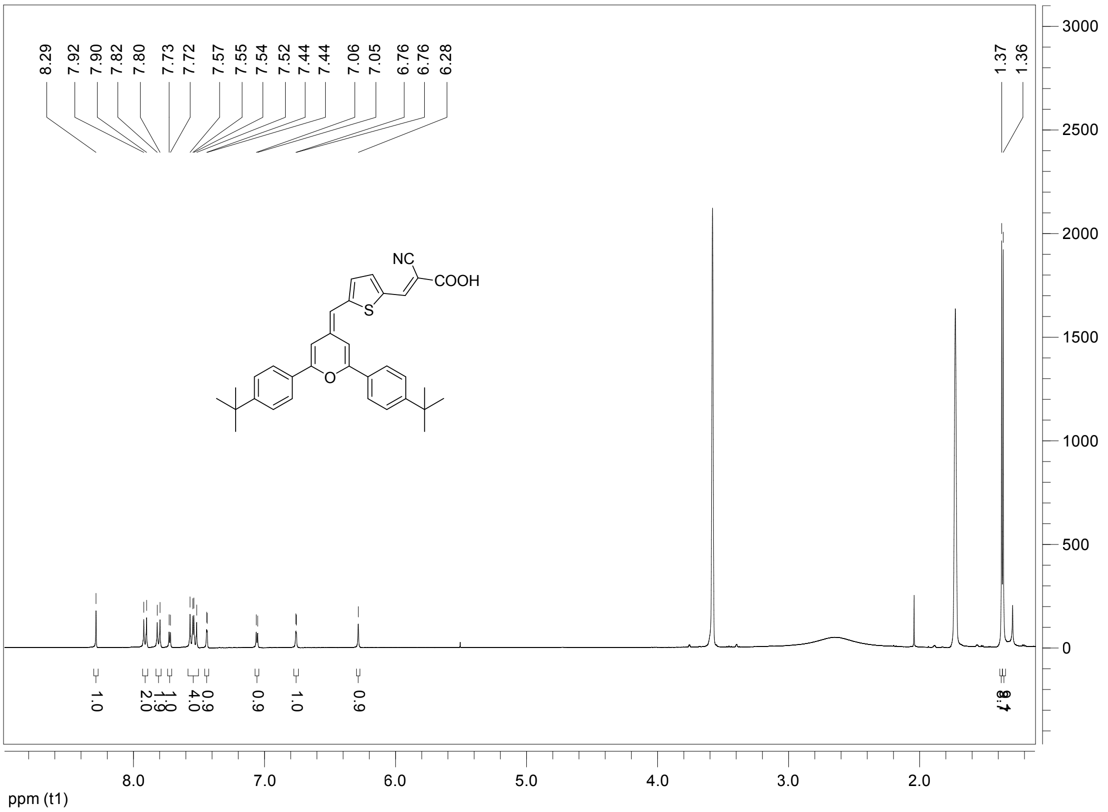


Figure S 11. *^{1}H-NMR spectrum of compound **9**.*

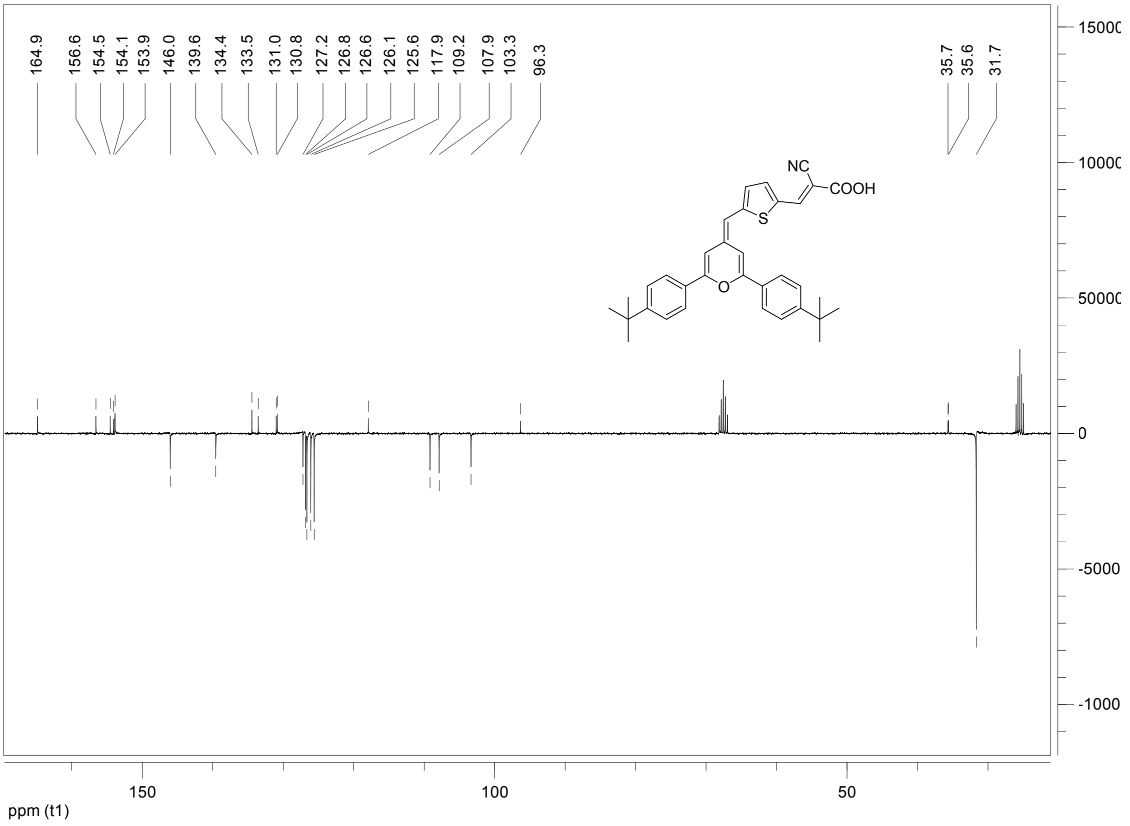


Figure S 12. *^{13}C-NMR spectrum of compound **9**.*

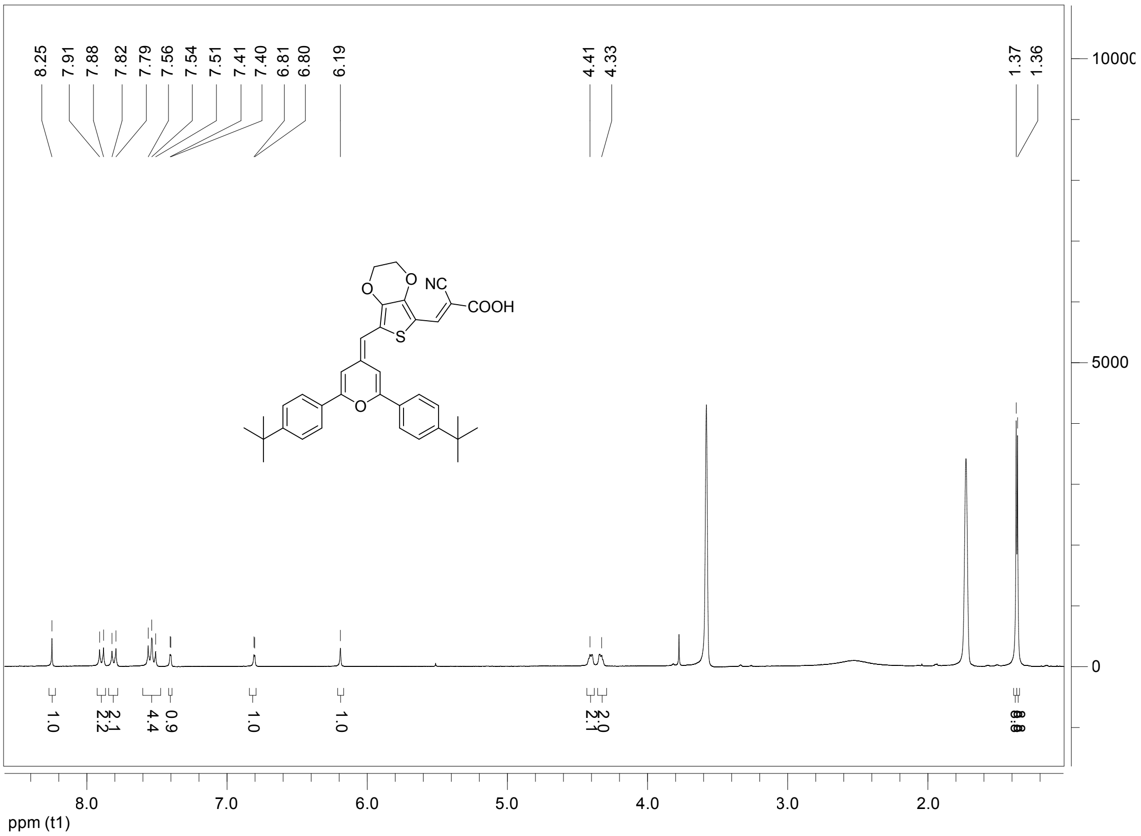


__Figure S 13.__ ^{1}H-NMR spectrum of compound __10__.

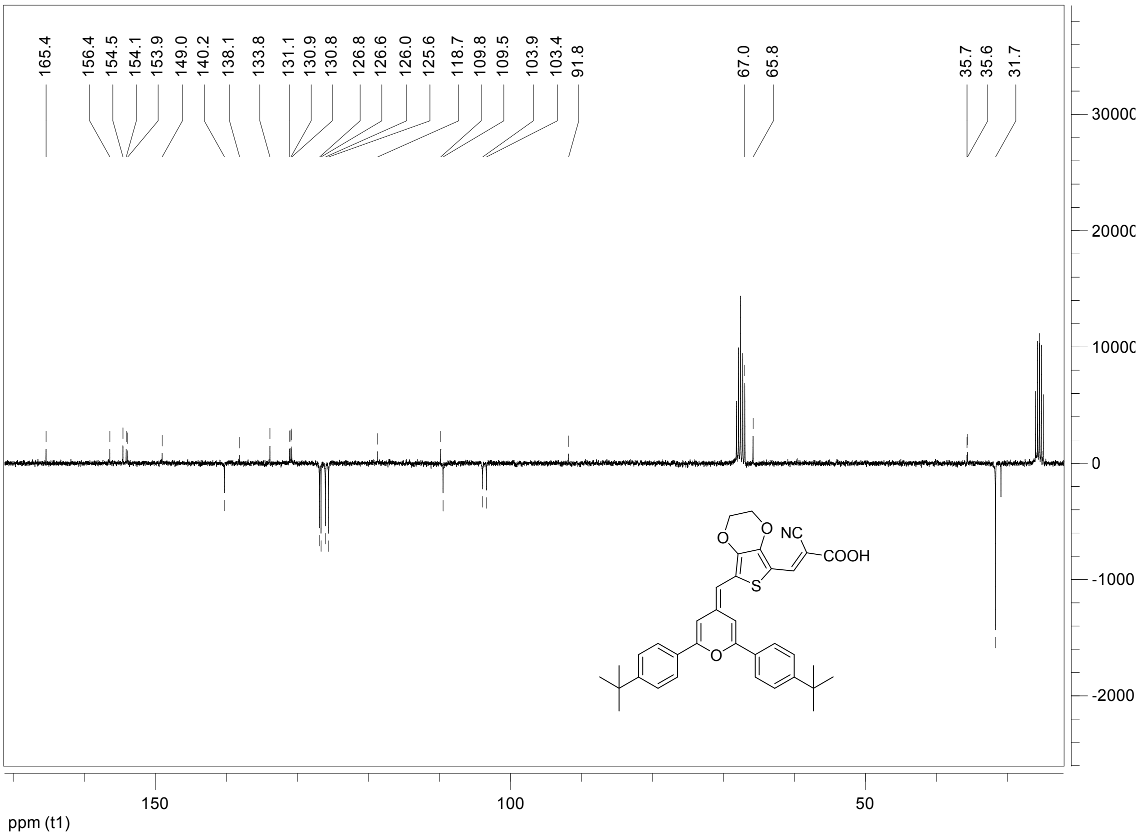


__Figure S 14.__ ^{13}C-NMR spectrum of compound __10__.

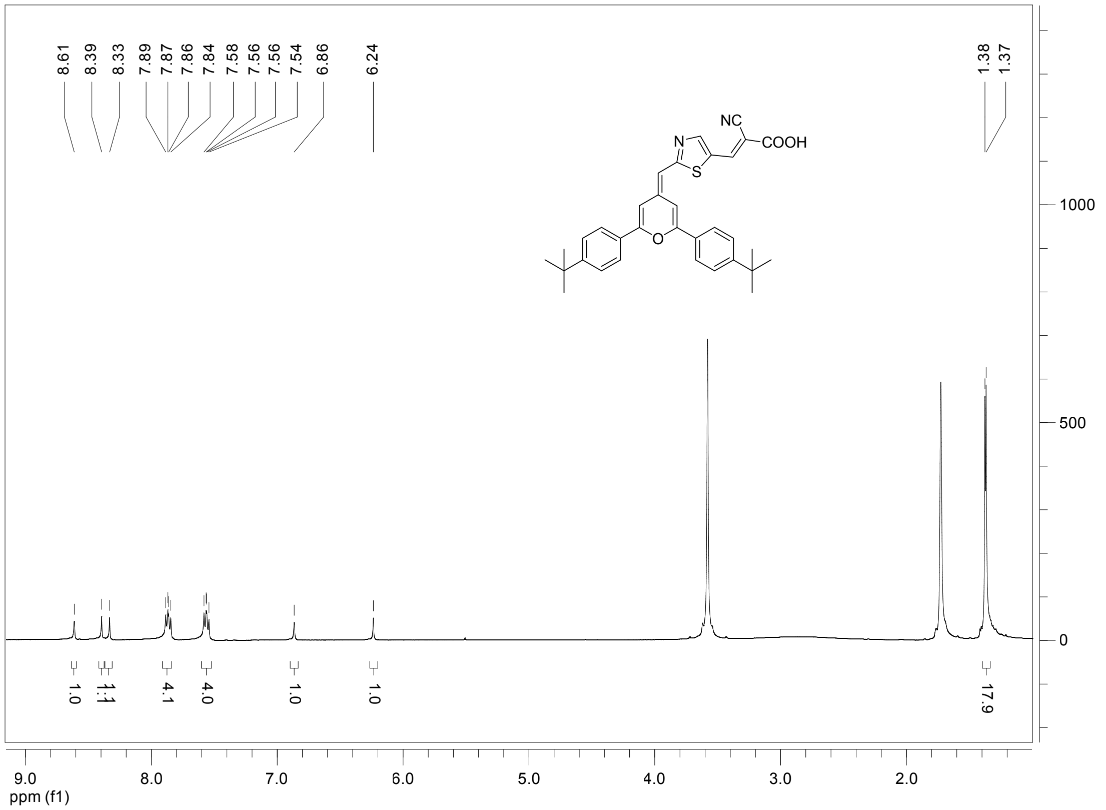


__Figure S 15.__ ^{1}H-NMR spectrum of compound __11__.

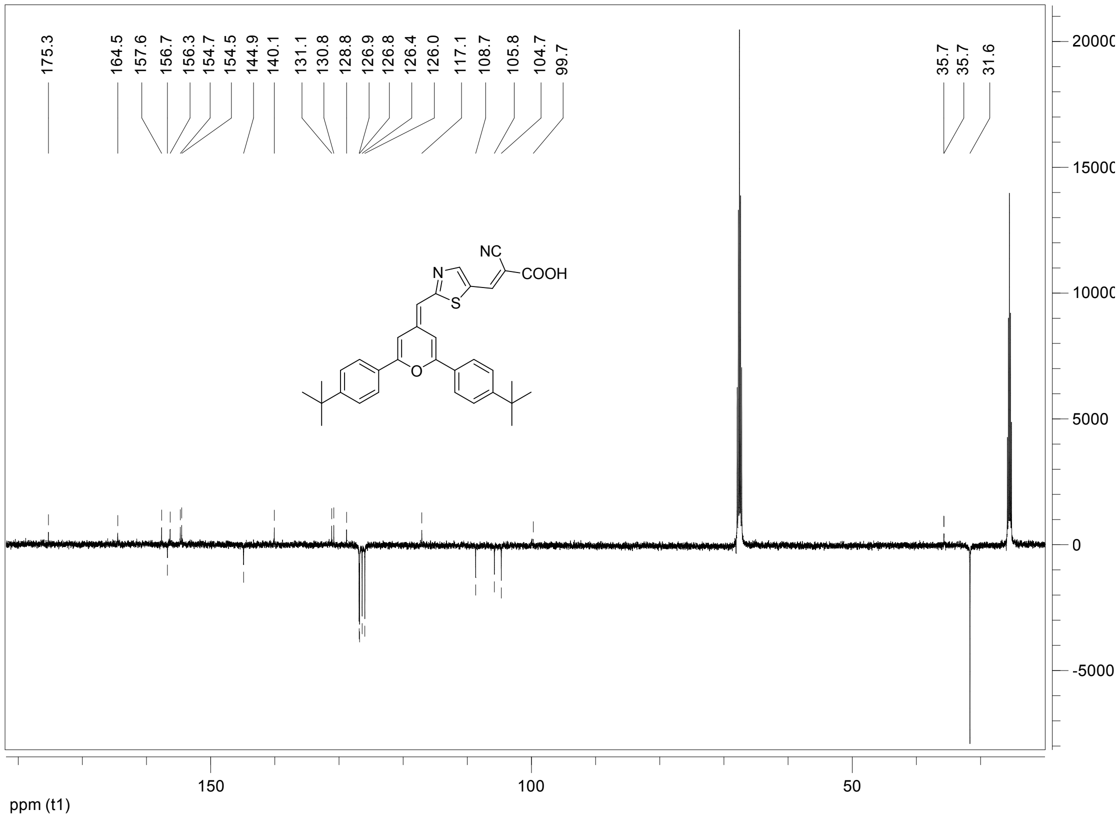


__Figure S 16.__ ^{13}C-NMR spectrum of compound __11__.

5. Mass Spectra

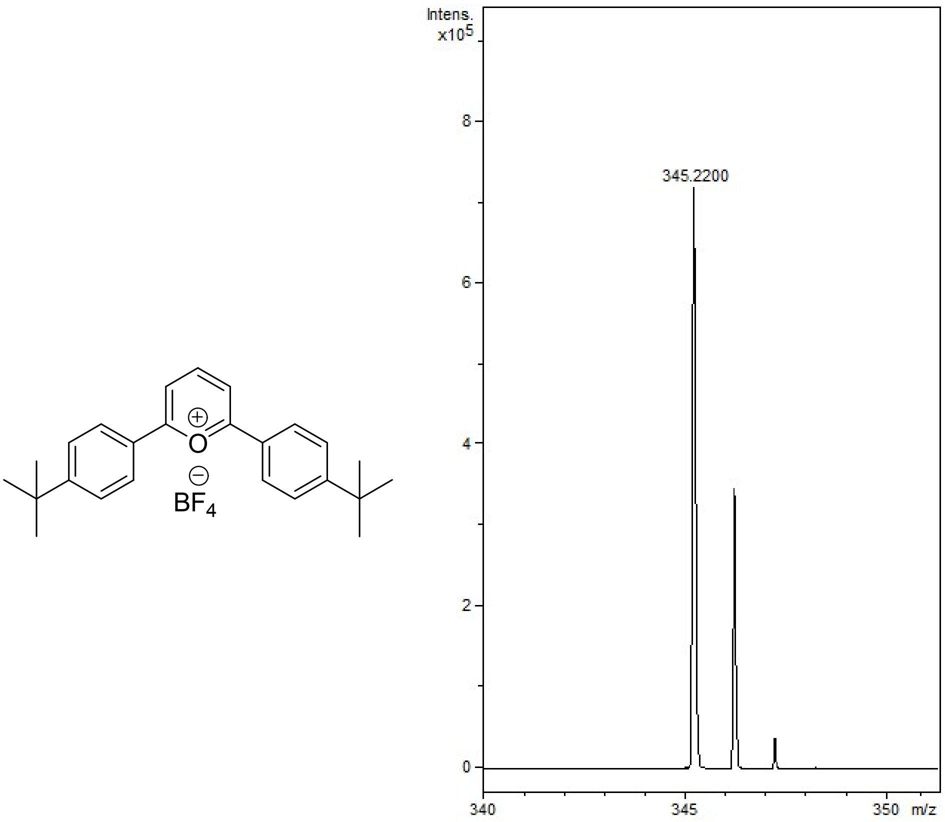


Figure S 17. *HRMS (ESI$^+$) spectrum of compound* ***1****.*

Figure S 18. *MS (MALDI$^+$) spectrum of compound* ***2****.*

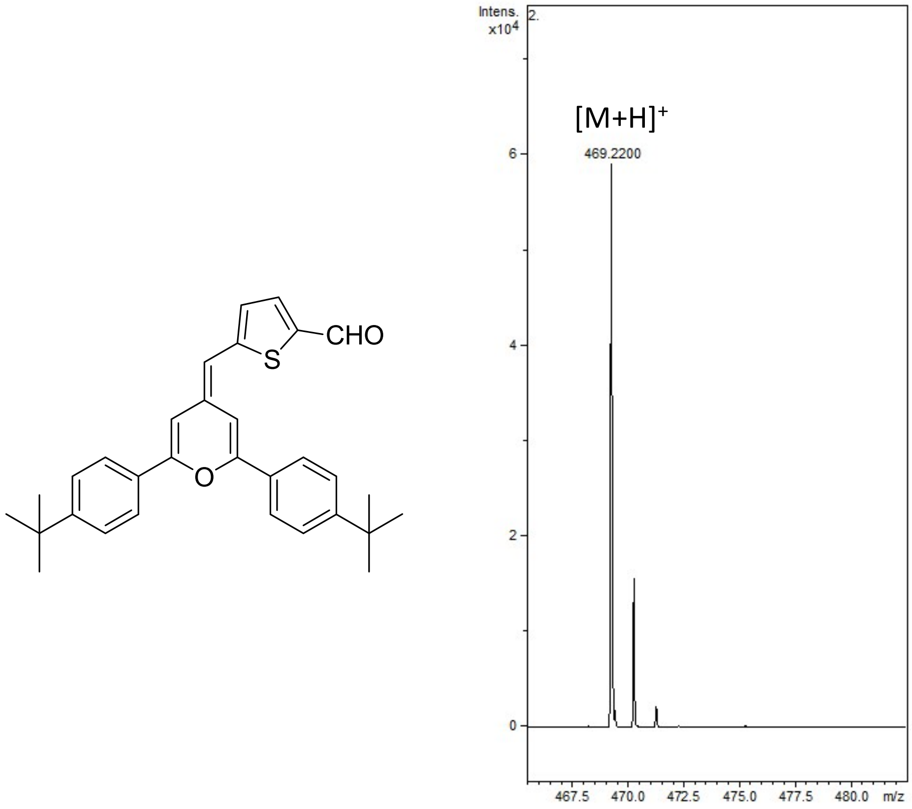


Figure S 19. *HRMS (ESI$^+$) spectrum of compound* ***6****.*

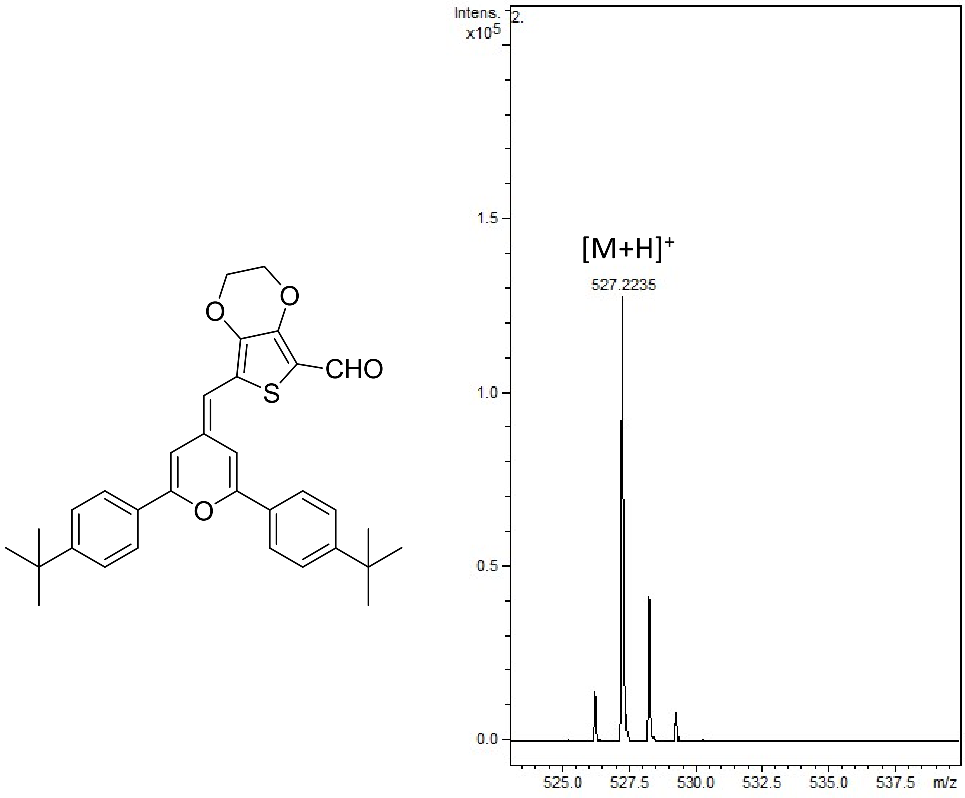


Figure S 20. *HRMS (ESI$^+$) spectrum of compound* ***7****.*

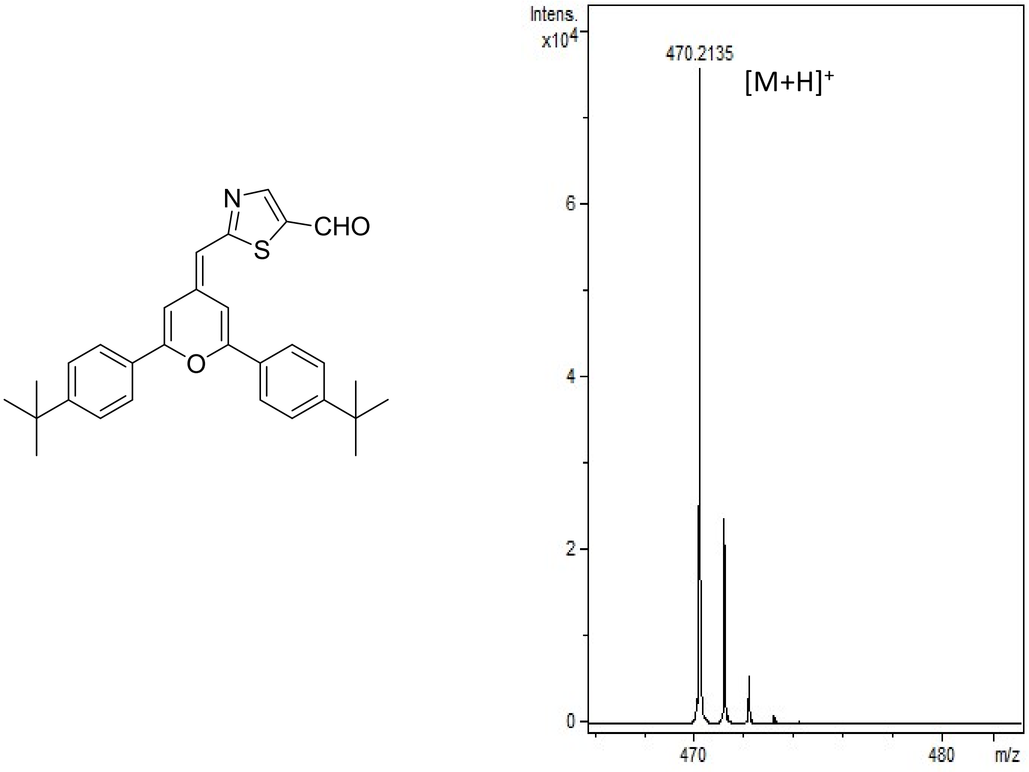


Figure S 21. *HRMS (ESI$^+$) spectrum of compound* ***8****.*

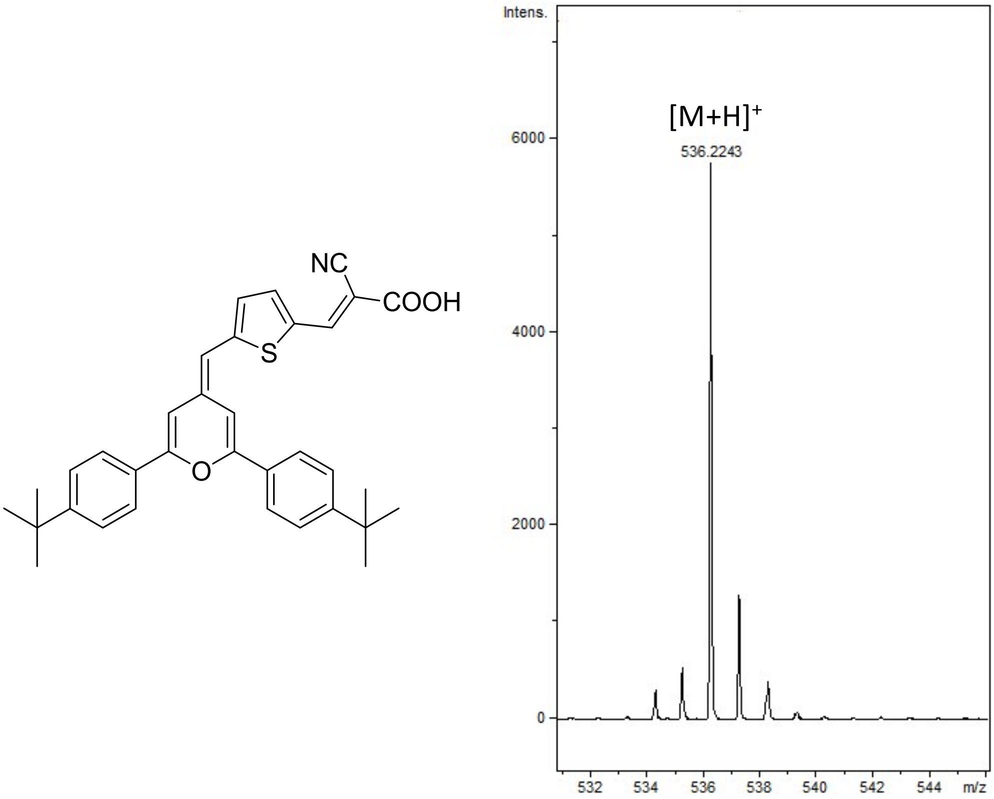


Figure S 22. *HRMS (ESI$^+$) spectrum of compound* ***9****.*

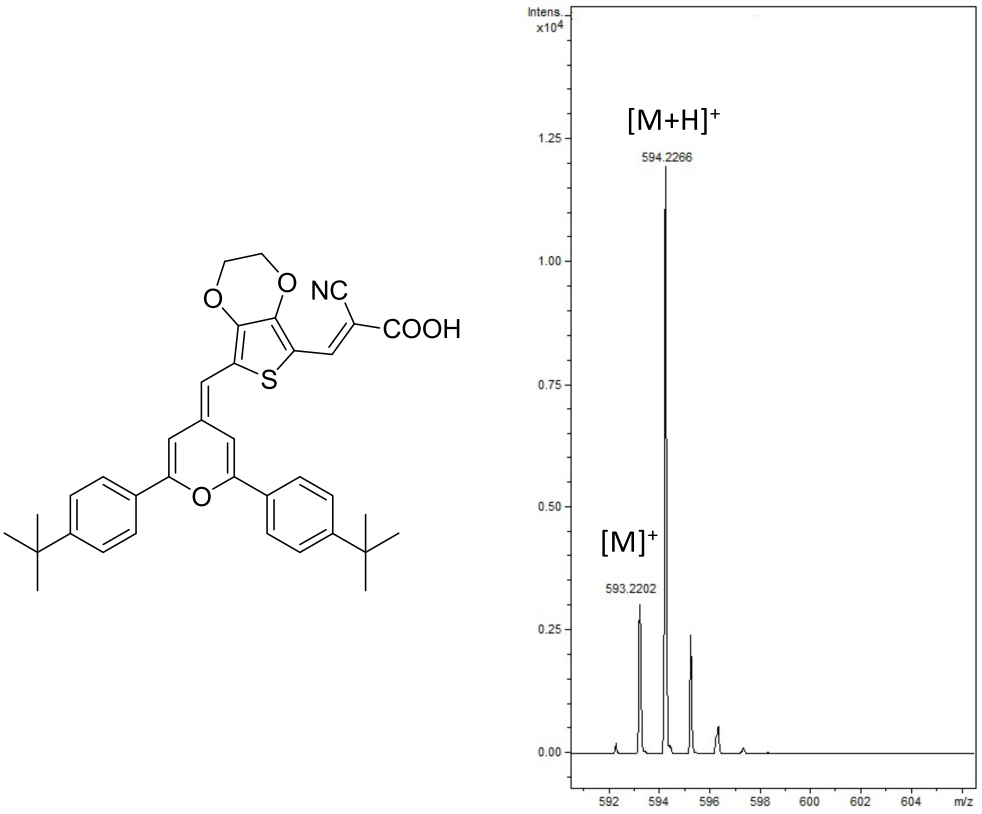


Figure S 23. *HRMS (ESI$^+$) spectrum of compound **10**.*

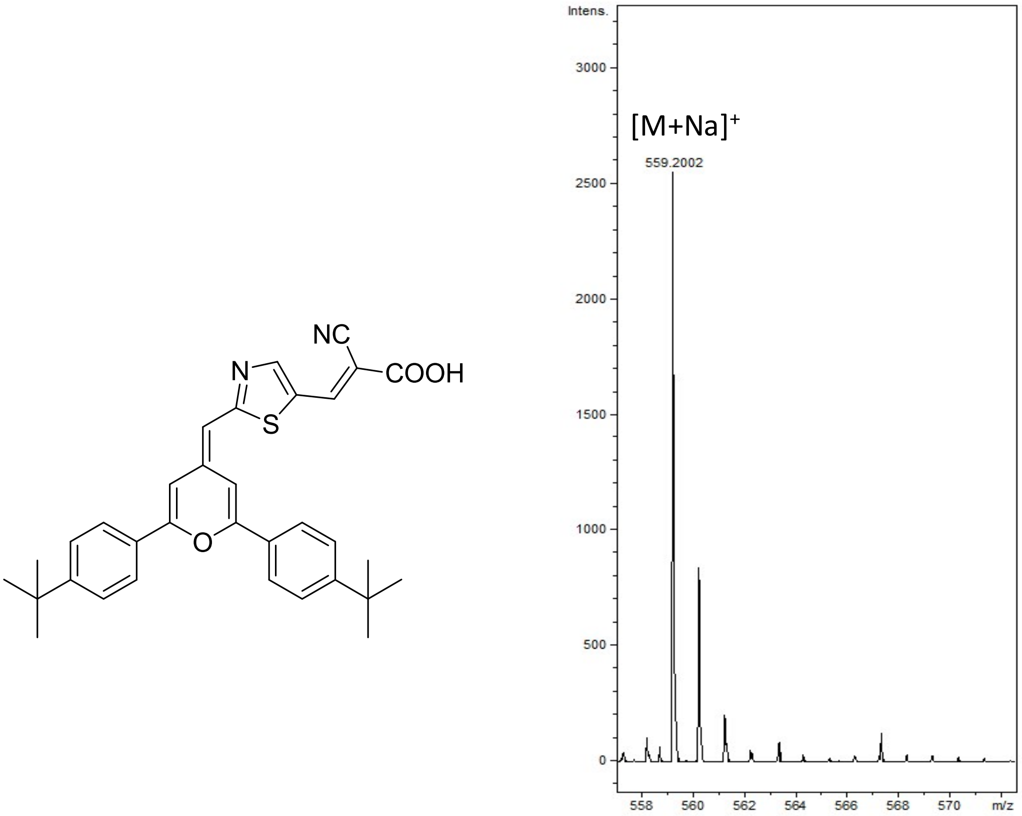


Figure S 24. *HRMS (ESI$^+$) spectrum of compound **11**.*

6. Differential pulse voltammograms

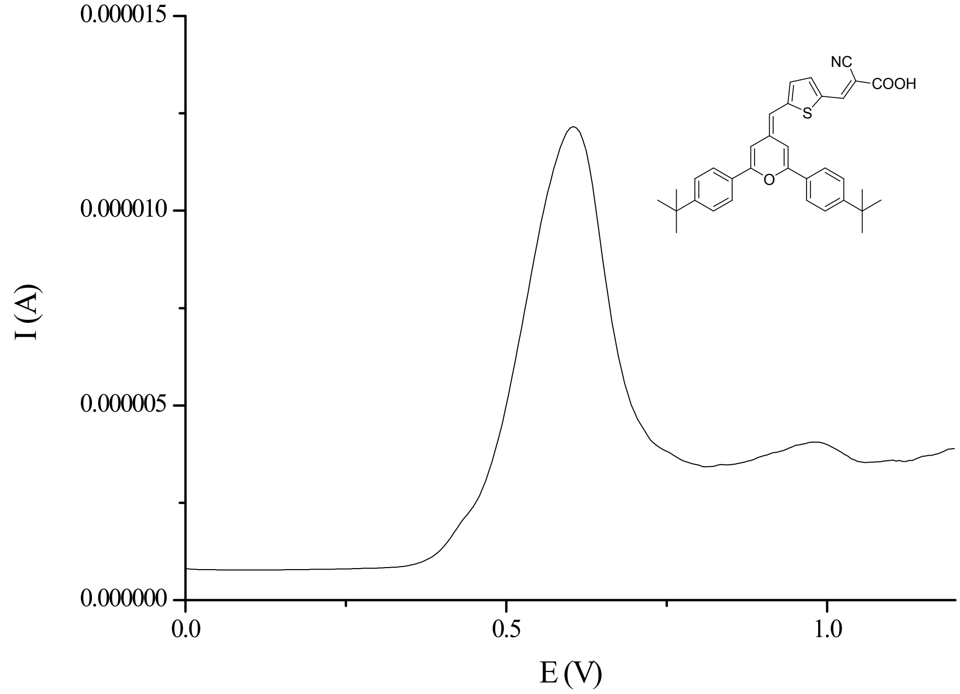


Figure S 25. *Differential pulse voltammogram of compound **9**.*

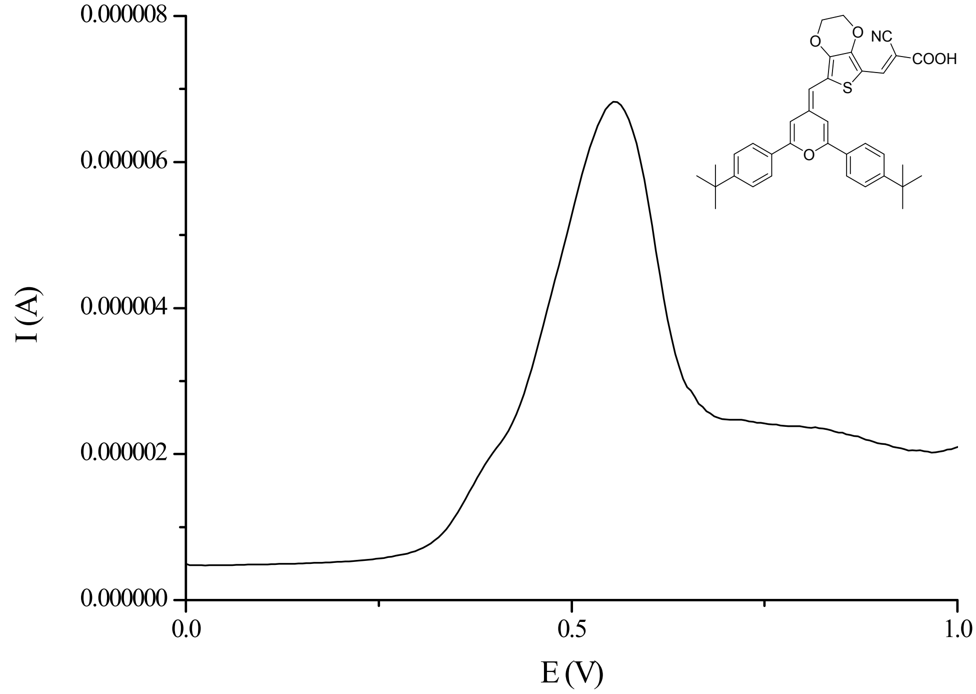


Figure S 26. *Differential pulse voltammogram of compound **10**.*

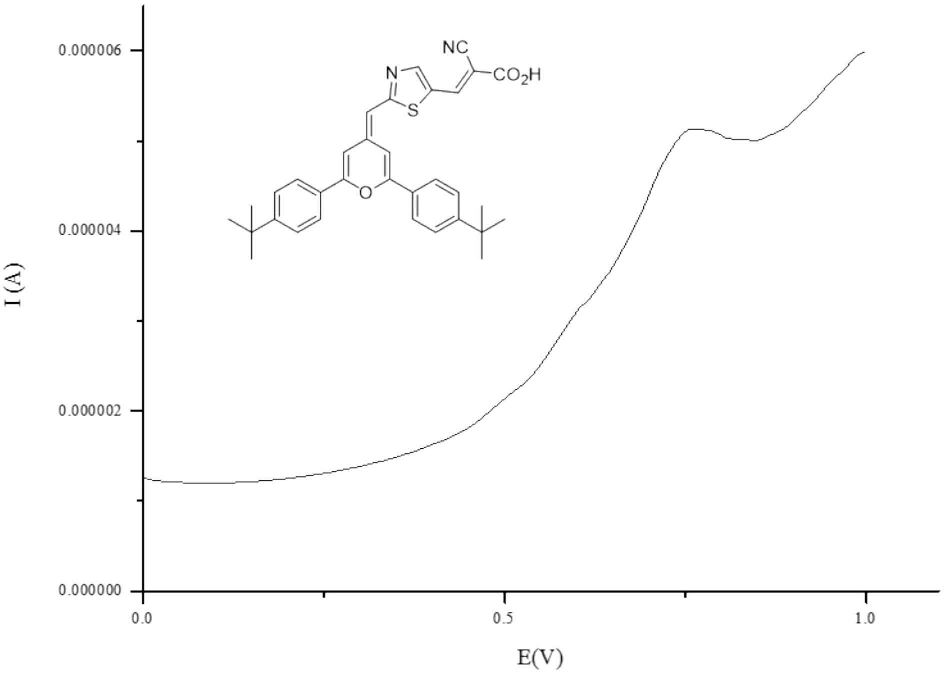


Figure S 27. *Differential pulse voltammogram of compound* ***11****.*

7. UV-Visible and emission spectra

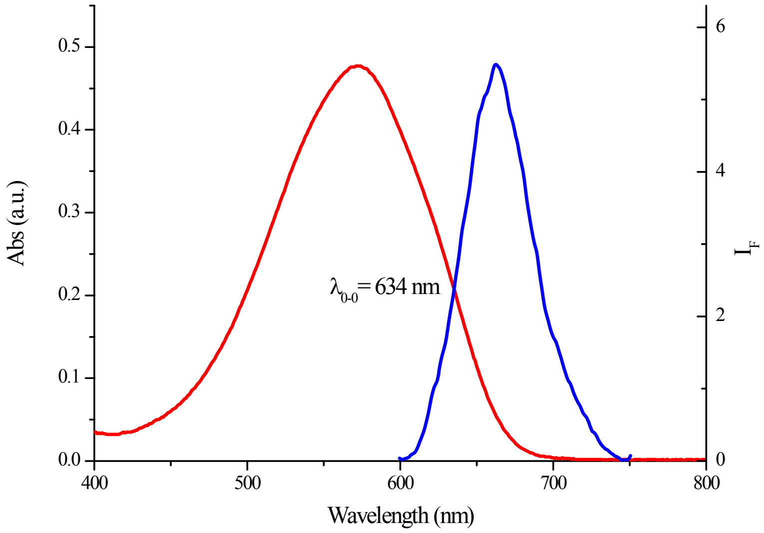


*Figure S 28. UV-Visible and emission spectra of compound **9**.*

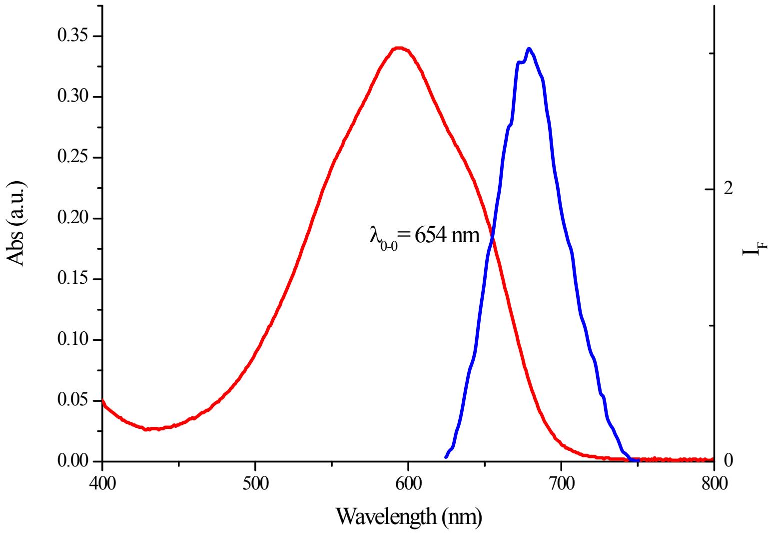


*Figure S 29. UV-Visible and emission spectra of compound **10**.*

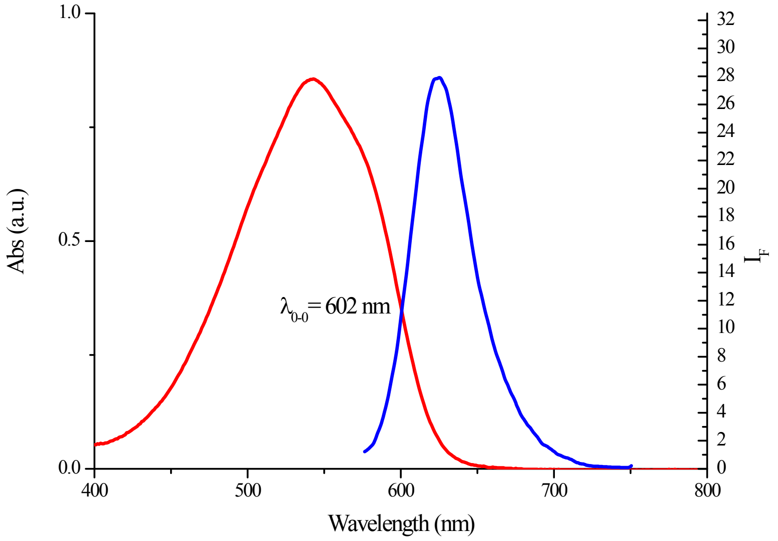
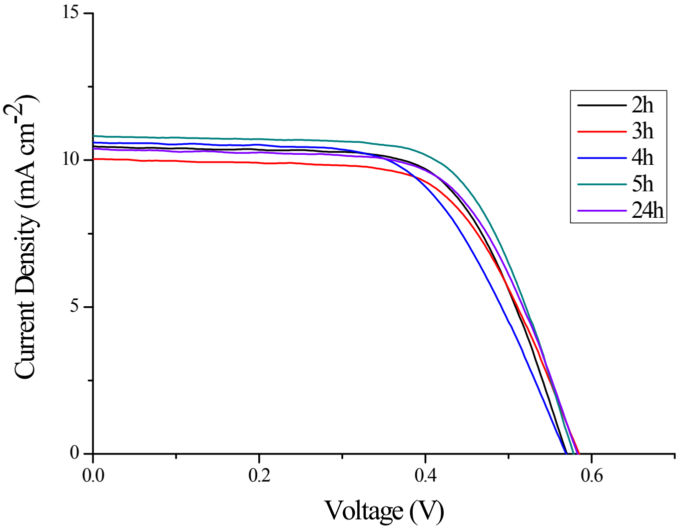


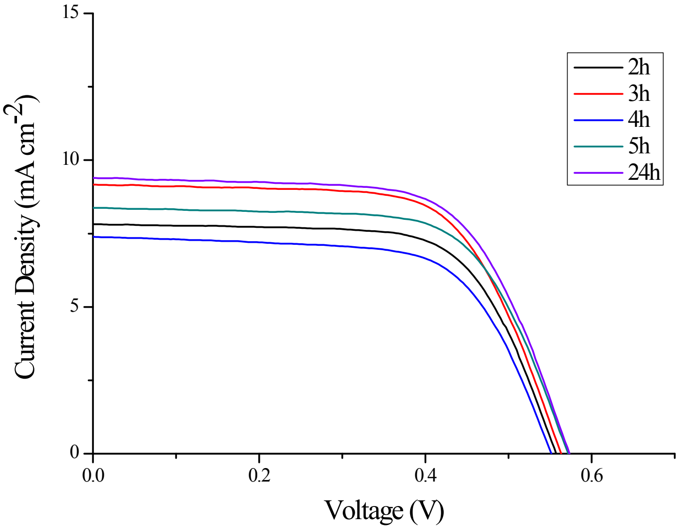
Figure S 30. *UV-Visible and emission spectra of compound* ***11****.*

8. J-V curves of the optimization process



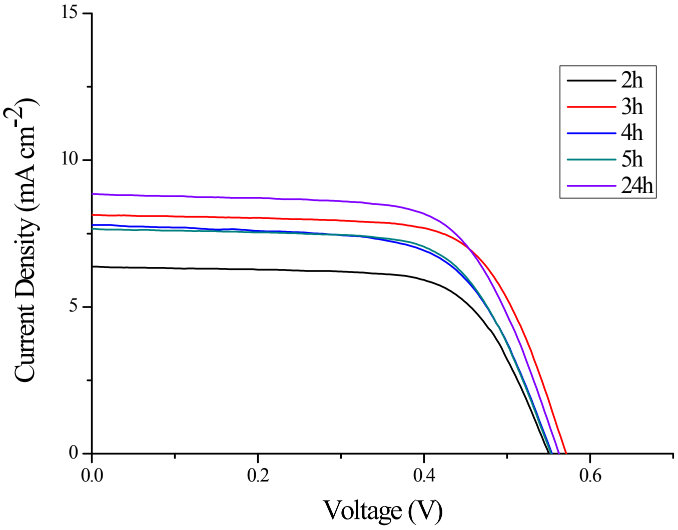
Time	J_{sc} (mA cm^{-2})	V_{oc} (V)	*ff* (%)	*η* (%)
2h	10.49	0.570	65.4	3.91
3h	10.06	0.584	63.5	3.73
4h	10.63	0.569	60.4	3.65
5h	10.84	0.578	66.3	4.15
24h	10.41	0.582	64.6	3.92

Figure S 31. *Photovoltaic measurements of compound* ***9*** *using 14 μm Solaronix anodes and* CH_2Cl_2 *as solvent for 5 different immersion times.*



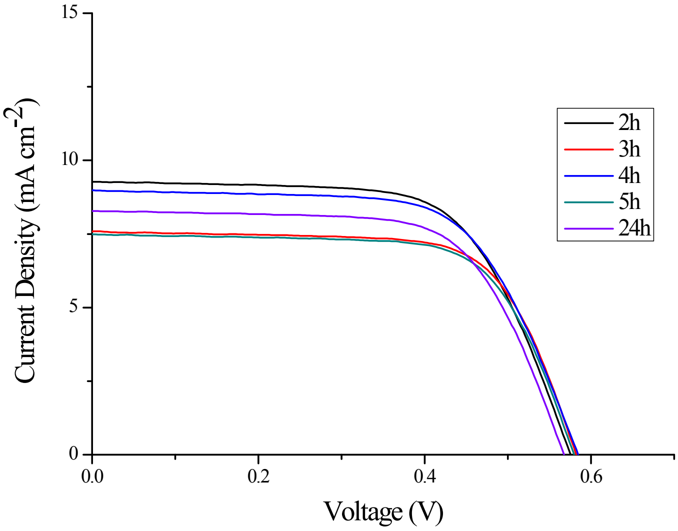
Time	J_{sc} (mA cm^{-2})	V_{oc} (V)	*ff* (%)	*η* (%)
2h	7.83	0.557	67.4	2.94
3h	9.19	0.563	65.9	3.41
4h	7.41	0.551	65.7	2.68
5h	8.39	0.571	66.8	3.20
24h	9.42	0.573	65.2	3.52

Figure S 32. *Photovoltaic measurements of compound* ***9*** *using 14 μm Solaronix anodes and acetonitrile/*^{t}*BuOH (1:1) as solvent for 5 different immersion times.*



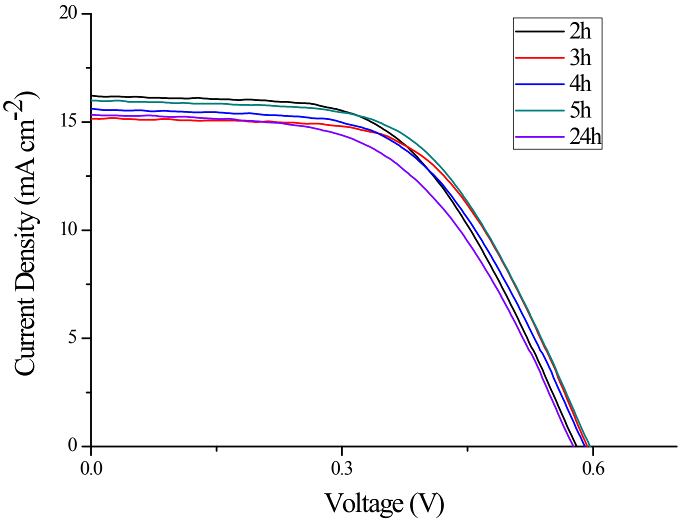
Time	J_{sc} (mA cm^{-2})	V_{oc} (V)	*ff* (%)	η (%)
2h	6.38	0.550	68.6	2.40
3h	8.15	0.571	68.8	3.20
4h	7.81	0.554	64.6	2.79
5h	7.67	0.552	67.1	2.84
24h	8.87	0.562	66.4	3.31

Figure S 33. *Photovoltaic measurements of compound **9** using 14 μm Solaronix anodes and THF as solvent for 5 different immersion times.*



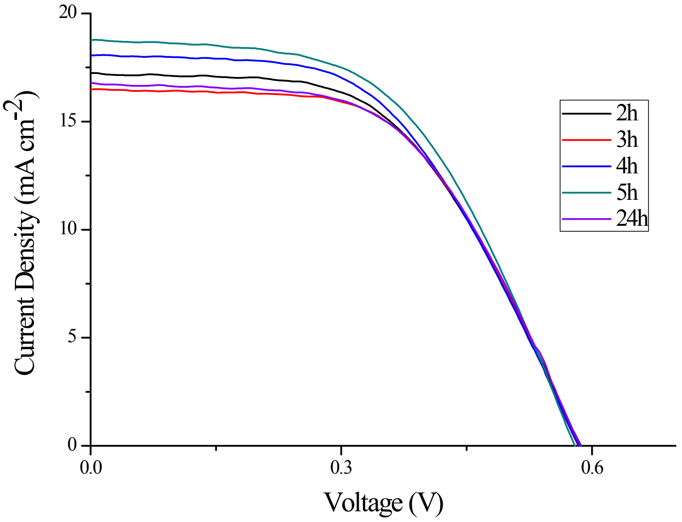
Time	J_{sc} (mA cm^{-2})	V_{oc} (V)	*ff* (%)	η (%)
2h	9.28	0.575	65.3	3.48
3h	7.59	0.582	69.1	3.05
4h	9.00	0.584	65.3	3.43
5h	7.50	0.579	69.0	2.99
24h	8.30	0.567	66.6	3.13

Figure S 34. *Photovoltaic measurements of compound **9** using 4 μm Solaronix anodes and CH_2Cl_2 as solvent for 5 different immersion times.*



Time	J_{sc} (mA cm^{-2})	V_{oc} (V)	*ff* (%)	η (%)
2h	16.20	0.580	55.7	5.23
3h	15.18	0.592	59.2	5.32
4h	15.60	0.590	56.3	5.18
5h	16.00	0.596	57.2	5.45
24h	15.35	0.575	54.2	4.79

Figure S 35. *Photovoltaic measurements of compound **9** using 4 μm Dyesol anodes and CH_2Cl_2 as solvent for 5 different immersion times.*



Time	J_{sc} (mA cm^{-2})	V_{oc} (V)	*ff* (%)	η (%)
2h	17.24	0.586	53.5	5.41
3h	16.52	0.583	56.0	5.39
4h	18.11	0.584	52.5	5.54
5h	18.79	0.579	53.4	5.80
24h	16.78	0.585	54.8	5.38

Figure S 36. *Photovoltaic measurements of compound **2** using 14 μm Dyesol anodes and CH_2Cl_2 as solvent for 5 different immersion times.*

9. References

1. A. K. Mohanakrishnan, A. Hucke, M. A. Lyon, M. V. Lakshmikantham and M. P. Cava, *Tetrahedron*, 1999, 55, 11745-11754.