

Molecular Engineering of Organic Dyes for Improved Recombination Lifetime in Solid-State Dye-Sensitized Solar Cells

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Supporting Information

1. Dye synthesis and characterization
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1. Dye synthesis and characterization

Methods

Materials

All chemicals and reagents, unless otherwise noted, were commercially sourced and used as received without further purification. D21L6 was used as received from Prof. Licheng Sun of KTH Royal Institute of Technology. C218 and Y123 were synthesized as previously reported.^{1,2}

Dry solvents were Acros AcroSeal Extra Dry solvents and used as received. Flash chromatography was performed using Silicycle P60 silica (60 Å pore size, 40 - 63 µm particle size distribution). 6-bromo-4,4'-dihexyl-9H-cyclopenta[2,1-*b*:3,4-*b'*]dithiophene-2-carbaldehyde was synthesized according to literature methods.¹

¹H and ¹³C NMR

¹H and ¹³C NMR spectra were collected in either DMSO-*d*₆ or dioxane-*d*₈ on a Varian Inova 500 MHz NMR spectrometer. Chemical shifts were determined relative to the solvent peak. DMSO: 2.50 ppm (¹H), 39.51 ppm (¹³C); dioxane: 3.53 ppm (¹H), 66.66 ppm (¹³C).

ESI-HRMS

ESI-HRMS data were collected at the Vincent Coates Foundation Mass Spectrometry Laboratory, Stanford University Mass Spectrometry (<http://mass-spec.stanford.edu>) with the assistance of Theresa Mary McLaughlin using a Micromass Q-ToF hybrid quadrupole-time of flight LC-MS. All ESI-HRMS samples were prepared in acetonitrile, with the exception of 7-bromo-9,9-dihexyl-*N,N*-bis(4-methoxyphenyl)-9H-fluoren-2-amine and bis(4-(hexyloxy)phenyl)amine, which were prepared in methanol. Samples were run by direct injection with a methanol carrier solvent and ionized using electrospray ionization.

Synthesis

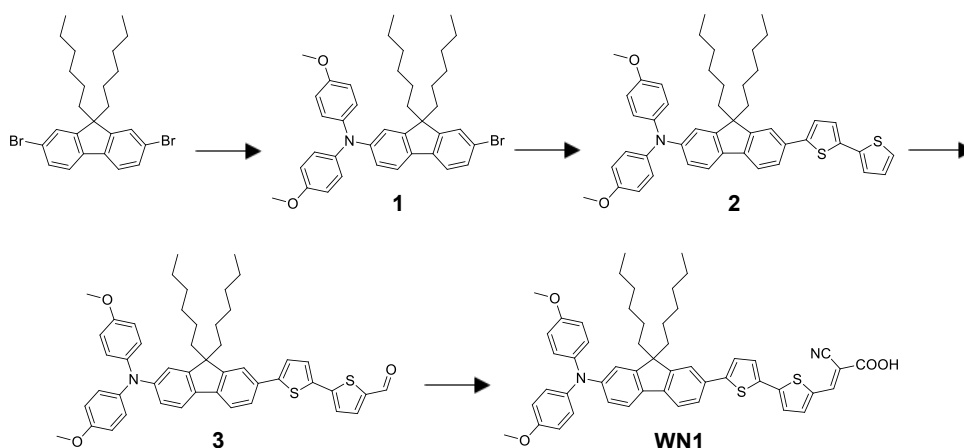


Figure S11. Synthetic scheme of **WN1**.

7-bromo-9,9-dihexyl-*N,N*-bis(4-methoxyphenyl)-9H-fluoren-2-amine (**1**): 4,4'-dimethoxydiphenylamine (1.9770 g, 8.623 mmol), 9,9-dihexyl-2,7-dibromofluorene (8.5002 g, 17.27 mmol), sodium *tert*-butoxide (1.7200 g, 17.90 mmol), 1,1'-bis(diphenylphosphino)ferrocene (0.0724 g, 0.131 mmol), bis(dibenzylideneacetone)palladium(0) (0.0776 g, 0.135 mmol), and a stir bar were charged into a 200 mL oven-dried Schlenk flask. The flask was evacuated and back-filled with nitrogen. 150 mL dry toluene was added and the reaction was stirred and heated at 80 °C for 22 h. The reaction was transferred to a round-bottom flask with hexane and ethyl acetate, and the solvent was removed by rotary evaporation. The resulting dark-brown oil was dissolved in methylene chloride and washed with water and brine. The organic layer was dried over magnesium sulfate

and filtered. The organic solvent was removed by rotary evaporation. The resulting brown oil was further purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford **1** as an off-white powder (4.0392 g, 73%). ¹H NMR (499.753 MHz, DMSO-*d*₆) δ 7.60 (m, 3H), 7.44 (dd, *J* = 8.0, 1.9 Hz, 1H), 6.97 (m, 4H), 6.88 (m, 5H), 6.75 (dd, *J* = 8.2, 2.1 Hz, 1H), 3.73 (s, 6H), 1.87 (m, 2H), 1.76 (m, 2H), 1.03 (m, 12H), 0.76 (t, *J* = 7.2 Hz, 6H), 0.52 (m, 4H) ppm; ¹³C NMR (125.674 MHz, DMSO-*d*₆) δ 155.4, 152.5, 151.1, 148.3, 140.6, 139.9, 132.6, 129.8, 125.8, 125.7, 120.9, 120.7, 120.0, 119.1, 115.4, 114.8, 55.2, 54.9, 30.8, 28.8, 23.3, 21.9, 13.9 ppm; HRMS (ESI) calcd. *m/z* for C₃₉H₄₆BrNO₂ [M]⁺. 639.2706, found 639.2714.

7-([2,2'-bithiophen]-5-yl)-9,9-dihexyl-*N,N*-bis(4-methoxyphenyl)-9*H*-fluoren-2-amine (**2**): bis(dibenzylideneacetone)palladium(0) (0.0394 g, 0.0685 mmol), tri-*o*-tolylphosphine (0.0225 g, 0.0739 mmol), and a stir bar were charged into an oven-dried 100 mL Schlenk flask. The flask was evacuated and back-filled with argon. A solution of 2,2'-bithiophene-5-boronic acid pinacol ester (0.5125 g, 1.754 mmol) and **1** (0.8947 g, 1.396 mmol) in 11 mL dry toluene was degassed with nitrogen in a scintillation vial and transferred to the Schlenk flask via syringe. The scintillation vial was rinsed with 15 mL dry toluene, and the rinsings were transferred to the Schlenk flask via syringe. A solution of tetraethylammonium hydroxide (20 wt. % in water) (3.25 mL, 4.458 mmol) was degassed with nitrogen and transferred to the Schlenk flask via syringe. The reaction was stirred and heated at 85°C for 22 h. The reaction was transferred to a round-bottom flask with hexane and ethyl acetate, and the solvent was removed by rotary evaporation. The resulting black, tar-like liquid was dissolved in a 2:3::hexane:ethyl acetate mixture and washed with 5% KOH_(aq.). The organic layer was then dried with Mg₂SO₄, filtered, and removed by rotary evaporation. The resulting brown-yellow oil was purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford a red-yellow solid. The solid was dissolved in methylene chloride and filtered to remove a few insoluble red solids. The solvent was removed by rotary evaporation to afford **2** as fine, yellow crystals (0.9698 g, 96%). ¹H NMR (499.753 MHz, DMSO-*d*₆) δ 7.64 (m, 2H), 7.59 (d, *J* = 8.3, 1H), 7.56 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.50 (m, 2H), 7.33 (dd, *J* = 3.5, 1.0 Hz, 1H), 7.31 (d, *J* = 3.8 Hz, 1H), 7.10 (dd, *J* = 5.0, 3.7 Hz, 1H), 6.98 (m, 4H), 6.90 (d, *J* = 2.0 Hz, 1H), 6.87 (m, 4H), 6.75 (dd, *J* = 8.3, 2.0 Hz, 1H), 3.73 (s, 6H), 1.90 (m, 2H), 1.76 (m, 2H), 1.02 (m, 12H), 0.73 (t, *J* = 7.1 Hz, 6H), 0.56 (m, 4H) ppm; ¹³C NMR (125.674 MHz, DMSO-*d*₆) δ 155.3, 151.6, 150.9, 148.0, 142.9, 140.6, 140.4, 136.5, 135.2, 133.3, 131.0, 128.4, 125.8, 125.4, 125.1, 124.3, 124.2, 123.9, 120.7, 120.0, 119.5, 119.2, 115.5, 114.8, 55.2, 54.6, 30.9, 28.8, 23.4, 21.9, 13.9 ppm; HRMS (ESI) calcd. *m/z* for C₄₇H₅₁NO₂S₂ [M]⁺. 725.3356, found 725.3364.

5'-(7-(bis(4-methoxyphenyl)amino)-9,9-dihexyl-9*H*-fluoren-2-yl)-[2,2'-bithiophene]-5-carbaldehyde (**3**): Compound **2** (0.2041 g, 0.2811 mmol) was charged into an oven-dried 25 mL Schlenk flask. The flask was evacuated and filled with argon. 3.5 mL dry DMF was added to the flask and the solution was stirred in an ice bath. 0.057 mL POCl₃ was added dropwise over 4 min. to a solution of 0.50 mL dry DMF under argon in an ice bath while stirring. The POCl₃ solution was stirred at room temperature for 40 min. producing a clear red solution. This solution was added to the reaction Schlenk flask dropwise via syringe over 5 min. while stirring in an ice bath. The reaction was stirred at room temperature for 1 h then heated to 70 °C for 24 h. The resulting opaque, deep-red solution was transferred to a round bottom flask with methylene

chloride and the solvent was removed by rotary evaporation leaving behind a dark-red oil. The oil was dissolved in methylene chloride and washed with 1 M KOH_(aq.) and brine. The organic layer was dried with Mg₂SO₄, filtered, and removed by rotary evaporation to produce a dark-red solid with a tinge of yellow. The solid was further purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford **3** as fine, pinkish-red crystals (0.0905 g, 43%). ¹H NMR (499.753 MHz, DMSO-*d*₆) δ 9.88 (s, 1H), 8.00 (d, J = 3.8 Hz, 1H), 7.70 (m, 1H), 7.66 (m, 1H), 7.61 (m, 4H), 7.54 (d, J = 4.2 Hz, 1H), 6.98 (m, 4H), 6.90 (d, J = 2.0 Hz, 1H), 6.87 (m, 4H), 6.75 (dd, J = 8.3, 1.8 Hz, 1H), 3.73 (s, 6H), 1.91 (m, 2H), 1.78 (m, 2H), 1.02 (m, 12H), 0.73 (t, J = 7.1 Hz, 6H), 0.56 (m, 4H) ppm; ¹³C NMR (125.674 MHz, DMSO-*d*₆) δ 183.7, 155.4, 151.7, 151.0, 148.2, 146.1, 145.6, 141.1, 141.0, 140.6, 139.3, 133.6, 133.1, 130.5, 128.3, 125.9, 124.9, 124.8, 124.6, 120.9, 119.9, 119.5, 119.5, 115.4, 114.8, 55.2, 54.6, 30.8, 28.8, 23.4, 21.9, 13.8 ppm; HRMS (ESI) calcd. m/z for C₄₈H₅₁NO₃S₂ [M]⁺ 753.3305, found 753.3302.

3-(5'-(7-(bis(4-methoxyphenyl)amino)-9,9-dihexyl-8*H*-fluoren-2-yl)-[2,2'-bithiophen]-5-yl)-2-cyanoacrylic acid (**WN1**): Compound **3** (0.3160 g, 0.4191 mmol), cyanoacetic acid (0.1176 g, 1.383 mmol), and a stir bar were charged into an oven-dried 100 mL Schlenk flask. The flask was evacuated and filled with nitrogen. 25 mL dry acetonitrile and piperidine (0.301 mL, 3.05 mmol) was added, and the reaction was stirred at 80 °C for 15 h. The reaction was transferred to a round bottom flask with methylene chloride and the solution was concentrated by rotary evaporation to approximately 10 mL. The concentrated solution was stirred with 50 mL 2M HCl_(aq.) five minutes. The organic layer was then washed with water and brine. The organic layer was dried with Mg₂SO₄, filtered, and removed by rotary evaporation to produce a metallic purple-black solid. The solid was further purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford a dark-red solid. The solid was dissolved in methylene chloride and washed with 2M HCl_(aq.) and brine. The organic layer was dried with Mg₂SO₄, filtered, and removed by rotary evaporation to afford **WN1** as a fine black powder (0.2964 g, 86%). ¹H NMR (499.753 MHz, DMSO-*d*₆) δ 8.49 (s, 1H), 7.99 (d, J = 4.4 Hz, 1H), 7.74 (m, 1H), 7.64 (m, 6H), 6.98 (m, 4H), 6.88 (m, 5H), 6.76 (dd, J = 8.3, 2.0 Hz, 1H), 3.74 (s, 6H), 1.94 (m, 2H), 1.78 (m, 2H), 1.04 (m, 12H), 0.74 (t, J = 7.1 Hz, 6H), 0.56 (m, 4H) ppm; ¹³C (125.674 MHz, DMSO-*d*₆) δ 163.7, 155.4, 151.8, 151.0, 148.2, 146.4, 145.8, 141.7, 141.1, 140.6, 133.8, 133.4, 133.1, 130.4, 128.5, 125.9, 125.0, 124.8, 124.7, 120.9, 119.9, 119.5, 116.7, 115.4, 114.8, 98.0, 55.2, 54.6, 30.9, 28.8, 23.4, 21.9, 13.9 ppm; HRMS (ESI) calcd. m/z for C₅₁H₅₂N₂O₄S₂ [M]⁺ 820.3363, found 820.3346.

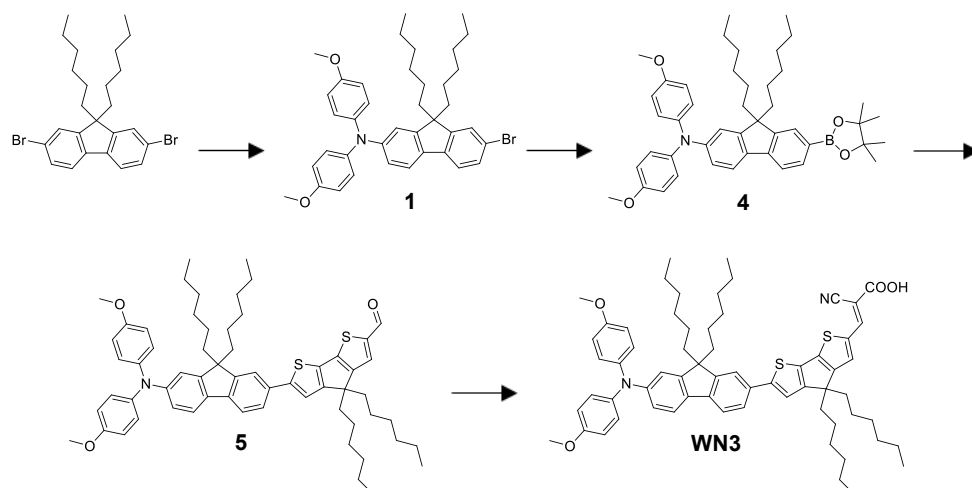


Figure SI2. Synthetic scheme of **WN3**.

7-bromo-9,9-dihexyl-*N,N*-bis(4-methoxyphenyl)-9*H*-fluorene-2-amine (**1**): Synthesized as reported above for **WN1**.

9,9-dihexyl-*N,N*-bis(4-methoxyphenyl)-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9*H*-fluorene-2-amine (**4**): Compound **2** (1.7817 g, 2.781 mmol), bis(pinacolato)diboron (0.9180 g, 3.615 mmol), [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium(II) (0.0832 g, 0.114 mmol), and KOAc (2.7514 g, 28.04 mmol) were charged into an oven-dried 100 mL Schlenk flask. The flask was evacuated and back-filled with nitrogen. 50 mL dry 1,4-dioxane was added and the reaction was stirred at 90 °C for 24 h, 100 °C for 4 h, and then 105 °C for 20 h. The reaction was dissolved in methylene chloride, filtered through filter paper, celite, and a fritted filter, and the solvent was removed by rotary evaporation leaving behind a black oil. The oil was purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford **4** as a fine pale-yellow powder (1.0367 g, 54%). ¹H NMR (499.753 MHz, DMSO-*d*₆) δ 7.61 (m, 4H), 6.98 (m, 4H), 6.90 (d, *J* = 2.2 Hz, 1H), 6.87 (m, 4H), 6.75 (dd, *J* = 8.2, 2.1 Hz, 1H), 3.73 (s, 6H), 1.80 (m, 4H), 1.30 (s, 12H), 1.02 (m, 12H), 0.75 (t, *J* = 7.1 Hz, 6H), 0.51 (m, 4H) ppm; ¹³C NMR (125.674 MHz, DMSO-*d*₆) δ 155.4, 151.9, 149.1, 148.4, 143.8, 140.6, 133.6, 133.3, 128.0, 125.8, 125.7, 121.1, 120.0, 118.4, 115.4, 114.8, 83.5, 55.2, 54.4, 30.8, 28.8, 24.8, 23.3, 21.9, 14.0 ppm; HRMS (ESI) calcd. *m/z* for C₄₅H₅₈BNO₄ [*M*]⁺ 687.4461, found 687.4468.

6-(7-(bis(4-methoxyphenyl)amino)-9,9-dihexyl-9*H*-fluorene-2-yl)-4,4-dihexyl-4*H*-cyclopenta[1,2-*b*:5,4-*b'*]dithiophene-2-carbaldehyde (**5**): Compound **4** (0.1080 g, 0.1570 mmol), tetrakis(triphenylphosphine)palladium(0) (0.0219 g, 0.0190 mmol), and a stir bar were charged into an oven-dried 50 mL Schlenk flask. The flask was evacuated and back-filled with nitrogen. A degassed solution of 4*H*-cyclopenta[2,1-*b*:3,4-*b'*]dithiophene-2-carbaldehyde (0.0879 g, 0.194 mmol) in 5 mL dry toluene was added to the reaction Schlenk flask via syringe along with two 2.5 mL dry toluene portions used to rinse the flask containing the solution of 4*H*-cyclopenta[2,1-*b*:3,4-*b'*]dithiophene-2-carbaldehyde. 5 mL degassed ethanol and degassed 5 M K₂CO_{3(aq.)} (0.377

mL, 1.87 mmol) were added via syringe. The reaction was stirred and heated at 78 °C for 14 h. The reaction was transferred to a round bottom flask with methylene chloride and water, and the solvent was removed by rotary evaporation, leaving behind white and bright-red solids. The solids were dissolved in methylene chloride and washed with water. The organic layer was dried with Mg₂SO₄, filtered through filter paper, celite, and a fritted filter, and the solvent was removed by rotary evaporation leaving behind a bright red solid. The solid was further purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford **5** as a fine, bright red-orange powder (0.1235 g, 84%). ¹H NMR (499.753 MHz, dioxane-*d*₈) δ 9.76 (s, 1H), 7.68 (s, 1H), 7.61 (m, 2H), 7.56 (m, 1H), 7.51 (d, J = 8.3 Hz, 1H), 7.36 (s, 1H), 7.04 (m, 4H), 6.67 (d, J = 2.0 Hz, 1H), 6.84 (m, 5H), 3.75 (s, 6H), 1.92 (m, 8H), 1.07 (m, 28H), 0.80 (m, 12H), 0.68 (m, 4H) ppm; ¹³C NMR (125.674 MHz, dioxane-*d*₈) δ 182.8, 163.8, 158.1, 156.8, 153.0, 152.2, 150.9, 149.6, 147.5, 144.8, 142.4, 142.2, 135.1, 134.5, 133.1, 130.3, 126.9, 125.4, 121.3, 121.3, 120.1, 120.0, 117.8, 116.8, 115.4, 55.8, 55.5, 54.9, 40.7, 38.6, 32.3, 32.2, 30.5, 30.4, 25.3, 24.5, 23.3, 23.3, 14.4, 14.4 ppm; HRMS (ESI) calcd. m/z for C₆₁H₇₅NO₃S₂ [M]⁺ 933.5183, found 933.5175.

3-(6-(7-(bis(4methoxyphenyl)amino)-9,9-dihexyl-9*H*-fluoren-2-yl)-4,4-dihexyl-4*H*-cyclopenta[1,2-*b*:5,4-*b'*]dithiophen-2-yl)-2-cyanoacrylic acid (**WN3**): Compound **5** (0.1028 g, 0.1100 mmol), cyanoacetic acid (0.0296 g, 0.3480 mmol), and a stir bar were charged into an oven-dried 50 mL Schlenk flask. The flask was evacuated and filled with nitrogen. 15 mL dry acetonitrile and piperidine (0.090 mL, 0.91 mmol) was added, and the reaction was stirred at 83 °C for 19 h. The reaction was transferred to a round bottom flask with methylene chloride and the solvent was removed by rotary evaporation leaving behind a red solid. The solid was dissolved in methylene chloride and washed with 2M HCl_(aq.). The organic layer was dried with Mg₂SO₄, filtered, and removed by rotary evaporation to produce a shiny purple-black solid. The solid was further purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford a purple-black solid. The solid was dissolved in methylene chloride and washed with 2M HCl_(aq.). The organic layer was dried with Mg₂SO₄, filtered, and removed by rotary evaporation to afford **WN3** as a fine black powder (0.1004 g, 91%). ¹H NMR (499.753 MHz, dioxane-*d*₈) δ 8.29 (s, 1H), 7.70 (m, 1H), 7.62 (m, 2H), 7.57 (m, 1H), 7.51 (d, J = 8.3 Hz, 1H), 7.37 (s, 1H), 7.04 (m, 4H), 6.97 (d, J = 2.2 Hz, 1H), 6.84 (m, 5H), 3.75 (s, 6H), 1.93 (m, 8H), 1.07 (m, 28H), 0.79 (m, 12H), 0.68 (m, 4H) ppm; ¹³C NMR (125.674 MHz, dioxane-*d*₈) δ 164.7, 164.5, 158.5, 156.8, 153.1, 152.3, 152.0, 149.8, 149.7, 147.7, 142.6, 142.2, 137.6, 135.3, 134.5, 133.0, 126.6, 125.6, 121.4, 121.3, 120.1, 120.0, 117.8, 117.6, 116.8, 115.435, 95.3, 55.8, 55.5, 54.8, 40.7, 38.6, 32.3, 32.2, 30.5, 30.4, 25.3, 24.6, 23.3, 23.3, 14.4, 14.4 ppm; HRMS (ESI) calcd. m/z for C₆₄H₇₆N₂O₄S₂ [M]⁺ 1000.5241, found 1000.5220.

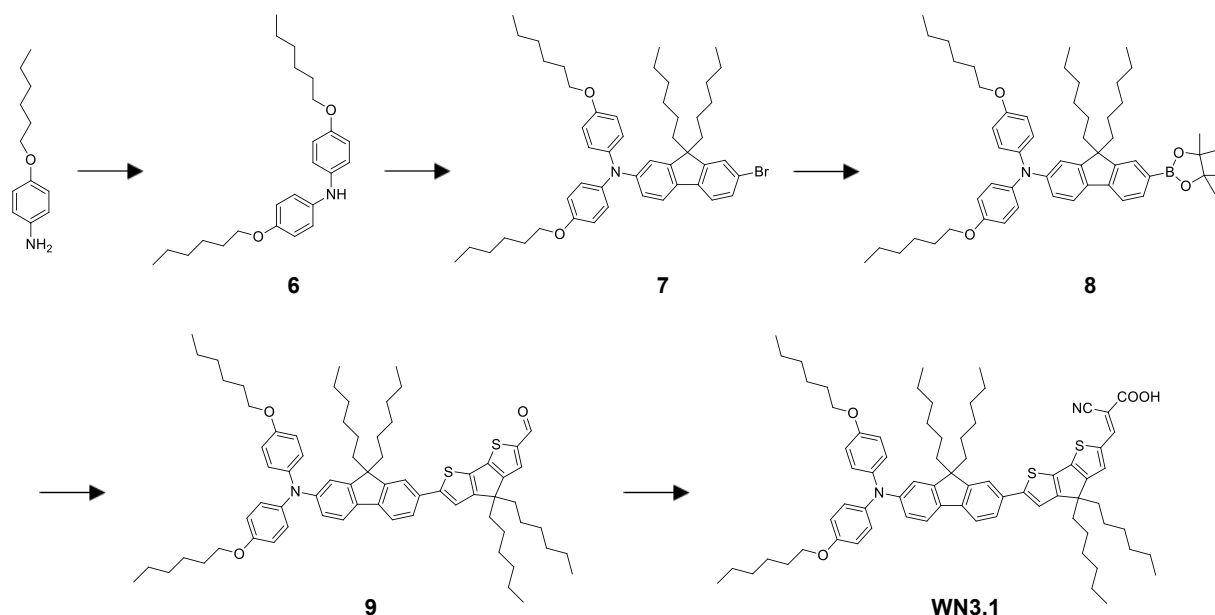


Figure SI3. Synthetic scheme of **WN3.1**.

bis(4-(hexyloxy)phenyl)amine (**6**): 4-(hexyloxy)aniline (0.7621 g, 3.943 mmol), 1,1'-bis(diphenylphosphino)ferrocene (0.0181 g, 0.0326 mmol), sodium *tert*-butoxide (0.3809 g, 3.964 mmol), bis(dibenzylideneacetone)palladium(0) (0.0199 g, 0.0346 mmol), and a stir bar were charged into an oven-dried 100 mL Schlenk flask. The flask was evacuated and filled with nitrogen. 50 mL dry toluene was added and the reaction was stirred for 1 h at room temperature. 1-bromo-4-(n-hexyloxy)benzene (0.520 mL, 1.969 mmol) was added via syringe and the reaction was stirred and heated to 80 °C for 22 h. The reaction was transferred to a round bottom flask with methylene chloride and the solvent was removed by rotary evaporation leaving behind a dark-brown oil with white solids. The oil was dissolved in methylene chloride and washed with water. The organic layer was reduced by rotary evaporation to a dark-brown solid. The solid was further purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford **6** as an off-white, fluffy powder (0.8413 g, 93%). ¹H NMR (125.674 MHz, DMSO-*d*₆) δ 7.50 (s, 1H), 6.88 (m, 4H), 6.79 (m, 4H), 3.86 (t, *J* = 6.5 Hz, 4H), 1.66 (m, 4H), 1.39 (m, 4H), 1.29 (m, 8H), 0.87 (m, 6H) ppm; ¹³C NMR (125.674 MHz DMSO-*d*₆) δ 152.2, 138.0, 118.0, 115.2, 67.7, 31.1, 28.8, 25.3, 22.1, 14.0 ppm; HRMS (ESI) caclcd. *m/z* for C₂₄H₃₆NO₂ [*M* + *H*]⁺ 370.2741, found 370.2726.

7-bromo-9,9-dihexyl-*N,N*-bis(4-(hexyloxy)phenyl)-9*H*-fluoren-2-amine (**7**): Compound **6** (2.2143 g, 5.992 mmol), 9,9-dihexyl-2,7-dibromofluorene (6.0571 g, 12.30 mmol), 1,1'-bis(diphenylphosphino)ferrocene (0.0512 g, 0.0924 mmol), bis(dibenzylideneacetone)palladium(0) (0.0543 g, 0.0944 mmol), sodium *tert*-butoxide (1.2723 g, 13.24 mmol), and a stir bar were charged into a 500 mL oven-dried Schlenk flask. The flask was evacuated and back-filled with nitrogen. 250 mL dry toluene was added and the reaction was stirred and heated at 80 °C for 23 h and 85 °C for 18 h. The reaction was transferred to a round-bottom flask with methylene chloride and water and the solvent was removed by rotary

evaporation. The resulting brown oil was dissolved in methylene chloride and washed with water. The organic layer was reduced by rotary evaporation to a clear, dark-brown oil. The resulting brown oil was further purified via column chromatography using an eluent of a gradient of increasing ethyl acetate concentration in hexane to afford **7** as a clear, light-yellow oil (3.6461 g, 78%). ¹H NMR (499.753 MHz, dioxane-*d*₈) δ 7.47 (m, 3H), 7.40 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.00 (m, 4H), 6.94 (d, *J* = 2.2 Hz, 1H), 6.80 (m, 5H), 3.91 (t, *J* = 6.3 Hz, 4H), 1.83 (m, 4H), 1.74 (m, 4H), 1.46 (m, 4H), 1.34 (m, 8H), 1.09 (m, 12H), 0.91 (m, 6H), 0.80 (t, *J* = 7.2 Hz, 6H), 0.61 (m, 4H) ppm; ¹³C NMR (125.674 MHz, dioxane-*d*₈) δ 156.2, 153.7, 152.4, 149.7, 142.1, 141.3, 134.0, 130.8, 126.9, 126.6, 121.3, 121.2, 121.1, 120.2, 116.7, 115.9, 68.6, 56.0, 40.5, 32.4, 32.2, 30.4, 30.1, 26.6, 24.5, 23.4, 23.3, 14.5, 14.4 ppm; HRMS (ESI) calcd. *m/z* for C₄₉H₆₆BrNO₂ [M]⁺ 779.4271, found 779.4261.

9,9-dihexyl-*N,N*-bis(4-(hexyloxy)phenyl)-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9*H*-fluoren-2-amine (**8**): Bis(pinacolato)diboron (1.5016 g, 5.913 mmol), [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium(II) (0.2685 g, 0.3632 mmol), and KOAc (1.8225 g, 18.57 mmol) were charged into an oven-dried 200 mL Schlenk flask. The flask was evacuated and back-filled with nitrogen. A degassed solution of **7** (3.5446 g, 4.539 mmol) in 15 mL dry 1,4-dioxane was added via syringe to the reaction flask along with five 15 mL dry 1,4-dioxane portions used to rinse the flask containing the solution of **7**. The reaction was stirred at 90 °C for 45 h. The reaction was transferred to a round-bottom flask with methylene chloride and water and the solvent was removed by rotary evaporation leaving behind a black oil. The oil was dissolved in methylene chloride and washed with water. The organic layer was reduced by rotary evaporation to a black oil. The oil loaded onto a column packed with oven dried silica and eluted using an eluent of a gradient of increasing methylene chloride concentration in hexane to afford **8** as a pale-yellow, sticky solid (3.1303 g, 83%). ¹H NMR (499.753 MHz, dioxane-*d*₈) δ 7.62 (m, 3H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.01 (m, 4H), 6.96 (d, *J* = 2.0 Hz, 1H), 6.83 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.79 (m, 4H), 3.91 (t, *J* = 6.5 Hz, 4H), 1.80 (m, 8H), 1.46 (m, 4H), 1.33 (m, 20H), 1.08 (m, 12H), 0.91 (m, 6H), 0.79 (t, *J* = 7.1 Hz, 6H), 0.59 (m, 4H) ppm; ¹³C NMR (125.674 MHz, dioxane-*d*₈) δ 156.1, 153.3, 150.3, 149.7, 145.2, 142.2, 135.0, 134.7, 129.2, 126.8, 121.6, 121.3, 118.9, 117.0, 115.9, 84.2, 68.6, 55.6, 40.6, 32.4, 32.2, 30.4, 30.1, 26.6, 25.3, 24.5, 23.4, 23.3, 14.5, 14.4 ppm; HRMS (ESI) calcd. *m/z* for C₅₅H₇₈BNO₄ [M]⁺ 827.6027, found 827.6026.

6-(7-(bis(4-(hexyloxy)phenyl)amino)-9,9-dihexyl-9*H*-fluoren-2-yl)-4,4-dihexyl-4*H*-cyclopenta[1,2-*b*:5,4-*b'*]dithiophene-2-carbaldehyde (**9**):

Tetrakis(triphenylphosphine)palladium(0) (0.0846 g, 0.0732 mmol) and a stir bar were charged into an oven-dried 100 mL Schlenk flask. The flask was evacuated and back-filled with nitrogen. A degassed solution of **8** (0.3998 g, 0.4828 mmol) in 5 mL dry toluene was added to the reaction Schlenk flask via syringe along with three 5 mL dry toluene portions used to rinse the flask containing the solution of **8**. A degassed solution of 4*H*-cyclopenta[2,1-*b*:3,4-*b'*]dithiophene-2-carbaldehyde (0.2665 g, 0.5877 mmol) in 5 mL dry toluene was added to the reaction Schlenk flask via syringe along with three 5 mL dry toluene portions used to rinse the flask containing the solution of 4*H*-cyclopenta[2,1-*b*:3,4-*b'*]dithiophene-2-carbaldehyde. 10 mL dry toluene, degassed 5 M K₂CO_{3(aq)} (1.16 mL, 5.80 mmol), and 25 mL dry ethanol were added via syringe to the reaction flask. The reaction was stirred and heated at 78 °C for 23 h. The reaction was transferred

to a round bottom flask with methylene chloride and water, and the solvent was removed by rotary evaporation, leaving behind white and bright-red solids and a black oil. This was dissolved in methylene chloride and washed with water. The organic layer was reduced by rotary evaporation leaving behind a black-yellow-red oil. The oil was purified via column chromatography using an eluent of a gradient of increasing methylene chloride concentration in hexane to afford a bright red solid. The solid was recrystallized in methanol to afford **9** as bright-orange, fine, needle-like crystals (0.4183 g, 81%). ¹H NMR (499.753 MHz, dioxane-*d*₈) δ 9.76 (s, 1H), 7.68 (s, 1H), 7.61 (m, 2H), 7.55 (s, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.36 (s, 1H), 7.02 (m, 4H), 6.97 (d, *J* = 2.2 Hz, 1H), 6.85 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.81 (m, 4H), 3.92 (t, *J* = 6.5 Hz, 4H), 1.92 (m, 8H), 1.75 (m, 4H), 1.47 (m, 4H), 1.35 (m, 8H), 1.13 (m, 24H), 0.99 (m, 4H), 0.91 (m, 6H), 0.80 (m, 12H), 0.68 (m, 4H) ppm; ¹³C NMR (125.674 MHz, dioxane-*d*₈) δ 182.8, 163.8, 158.1, 156.3, 153.0, 152.3, 150.9, 149.7, 147.5, 144.8, 142.4, 142.1, 135.1, 134.4, 133.0, 130.3, 126.9, 125.4, 121.3, 121.2, 120.1, 120.0, 117.7, 116.8, 115.9, 68.6, 55.8, 54.9, 40.7, 38.6, 32.4, 32.3, 32.2, 30.5, 30.4, 30.1, 26.6, 25.3, 24.6, 23.4, 23.3, 14.5, 14.4, 14.4 ppm; HRMS (ESI) calcd. *m/z* for C₇₁H₉₅NO₃S₂ [M]⁺ 1073.6748, found 1073.6771.

3-(6-(7(bis(4-(hexyloxy)phenyl)amino)-9,9-dihexyl-9*H*-fluoren-2-yl)-4,4-dihexyl-4*H*-cyclopenta[1,2-*b*:5,4-*b'*]dithiophen-2-yl)-2-cyanoacrylic acid (**WN3.1**): Compound **9** (0.1363 g, 0.1268 mmol) and a stir bar were charged into an oven-dried 50 mL Schlenk flask. The flask was evacuated and filled with nitrogen. 25 mL dry acetonitrile was added via syringe. Cyanoacetic acid (0.0390 g, 0.459 mmol) was added to the flask under a flow of nitrogen. 7 mL dry methylene chloride and piperidine (0.091 mL, 0.92 mmol) were added via syringe, and the reaction was stirred at 85 °C for 18 h. Cyanoacetic acid (0.0220 g, 0.259 mmol) was added to the flask under a flow of nitrogen, and piperidine (0.040 mL, 0.40 mmol) was added via syringe. The reaction was stirred at 75 °C for an additional 24 h. The reaction was transferred to a round bottom flask with methylene chloride and the solvent was removed by rotary evaporation leaving behind a dark-red solid. The solid was dissolved in methylene chloride and washed with 2M HCl_(aq.). The organic layer was reduced by rotary evaporation to produce a dark-purple oil. The oil was loaded onto a column packed with silica and 1:1::ethyl acetate:hexane and eluted with a gradient of increasing methanol concentration in ethyl acetate to afford a red solid. The solid was dissolved in methylene chloride and washed with 2M HCl_(aq.). The organic layer reduced by rotary evaporation to afford **WN3.1** as a fine, black, shiny powder (0.1121 g, 77%). ¹H NMR (499.753 MHz, dioxane-*d*₈) δ 8.29 (s, 1H), 7.70 (s, 1H), 7.61 (m, 2H), 7.56 (s, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.37 (s, 1H), 7.02 (m, 4H), 6.97 (d, *J* = 2.0 Hz, 1H), 6.85 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.81 (m, 4H), 3.92 (t, *J* = 6.5 Hz, 4H), 1.92 (m, 8H), 1.75 (m, 4H), 1.47 (m, 4H), 1.35 (m, 8H), 1.13 (m, 24H), 0.99 (m, 4H), 0.91 (m, 6H), 0.80 (m, 12H), 0.68 (m, 4H) ppm; ¹³C NMR (125.674 MHz, dioxane-*d*₈) δ 164.7, 164.5, 158.5, 156.3, 153.0, 152.3, 152.1, 149.8, 149.7, 147.7, 142.6, 142.1, 137.5, 135.2, 134.4, 132.9, 131.8, 126.9, 125.6, 121.4, 121.2, 120.1, 120.0, 117.8, 117.6, 116.7, 115.9, 95.2, 68.6, 55.8, 54.8, 40.7, 38.6, 32.4, 32.3, 32.2, 30.5, 30.4, 30.1, 26.6, 25.3, 24.6, 23.4, 23.3, 23.3, 14.5, 14.4, 14.4 ppm; HRMS (ESI) calcd. *m/z* for C₇₄H₉₆N₂O₄S₂ [M]⁺ 1140.6806, found 1140.6813.

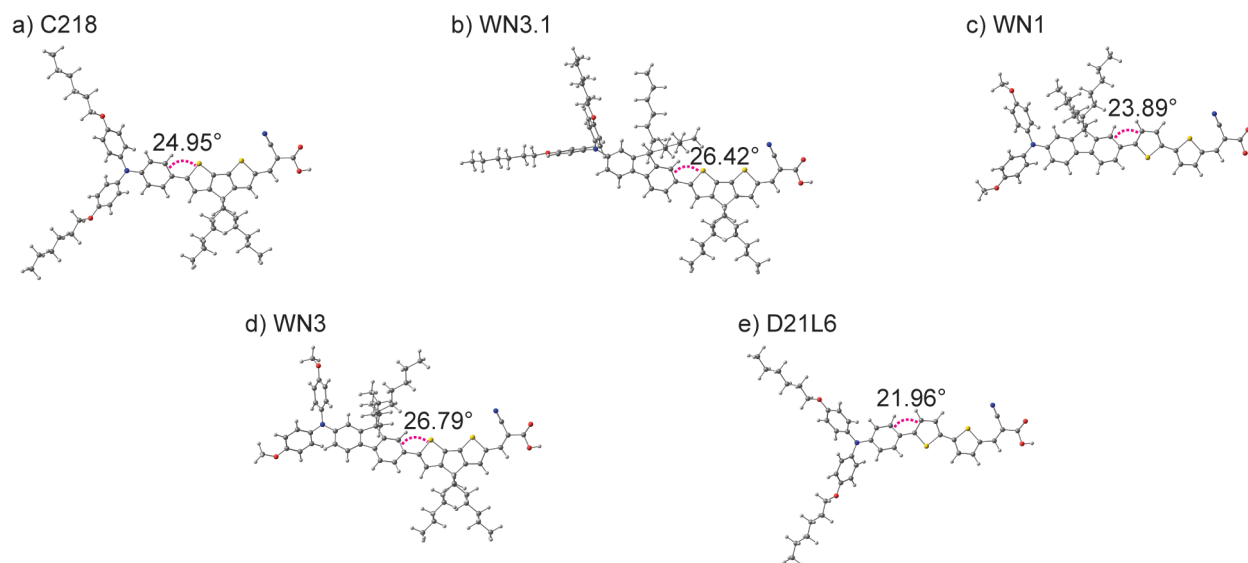


Figure SI4. Dihedral angle between a) phenyl and fused bithiophene π -groups or fluorene and fused bithiophene π -groups of a) C218, b) WN3.1, c) WN1, d) WN3, and e) D21L6 as determined from the optimized gas-phase geometry using density functional theory, performed with Gaussian09 and a B3LYP/6-31G* basis set.

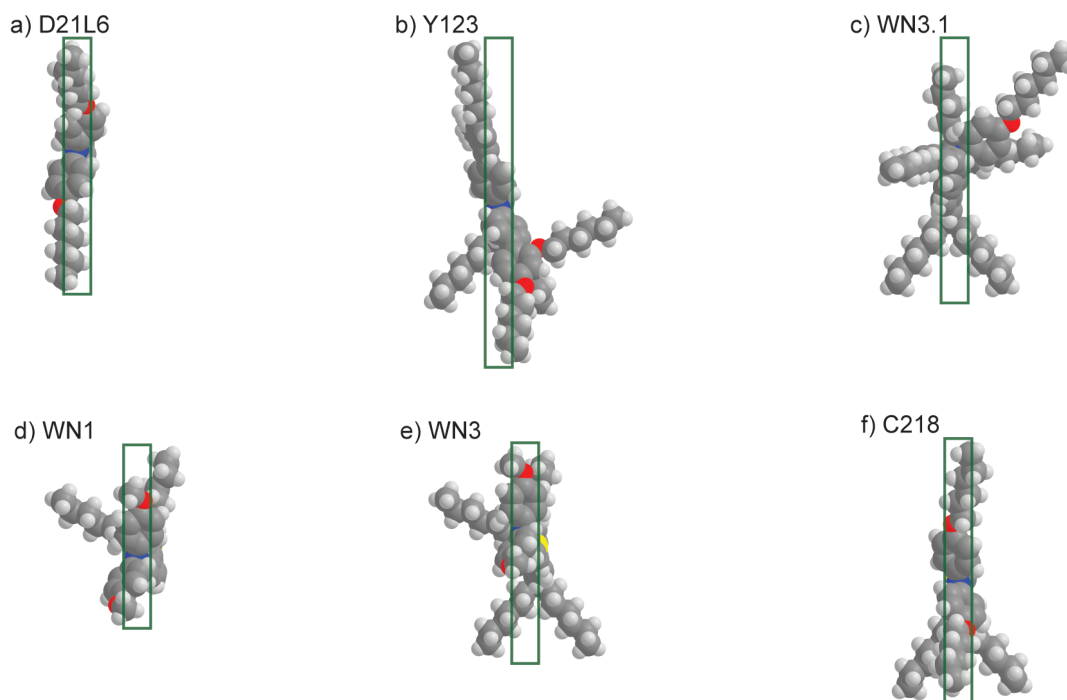


Figure SI5. Top-down, donor-to-acceptor, perspective of a) D21L6, b) Y123, c) WN3.1, d) WN1, e) WN3, and f) C218, as defined by the green arrow in Figure SI6; the green box indicates the conjugation plane along the π -backbone of the dye.

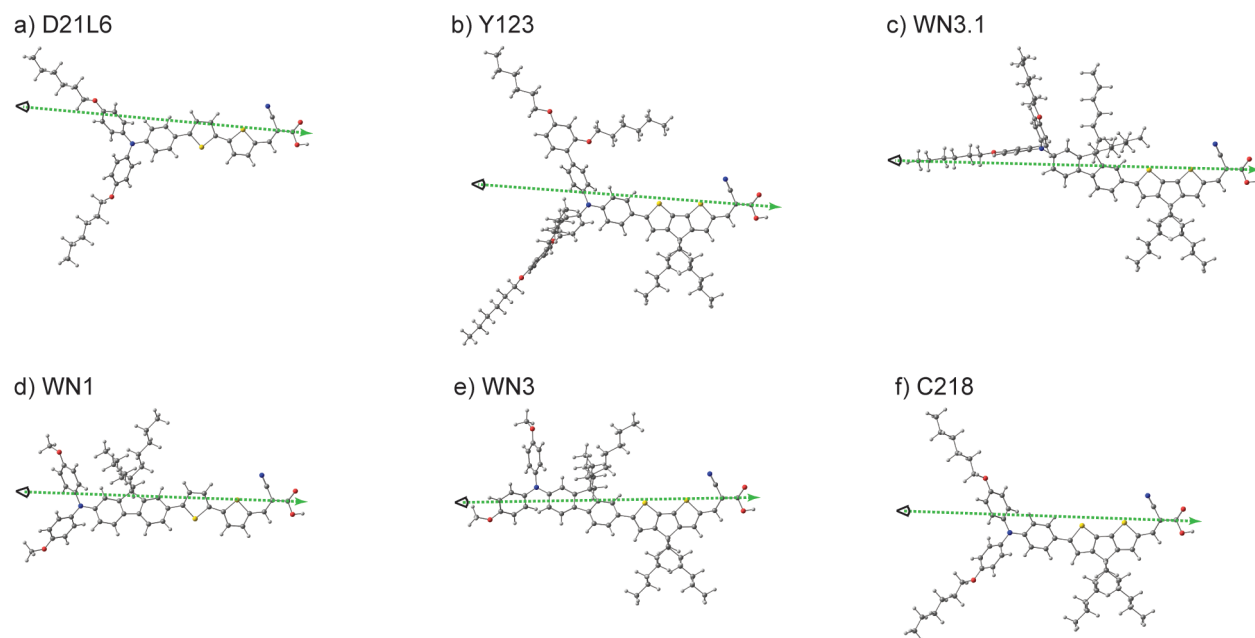
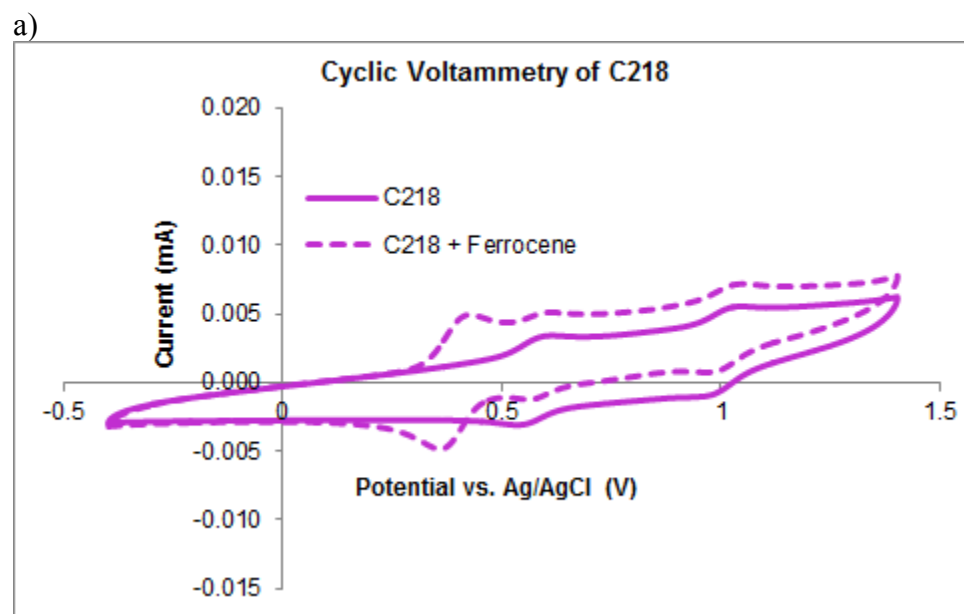
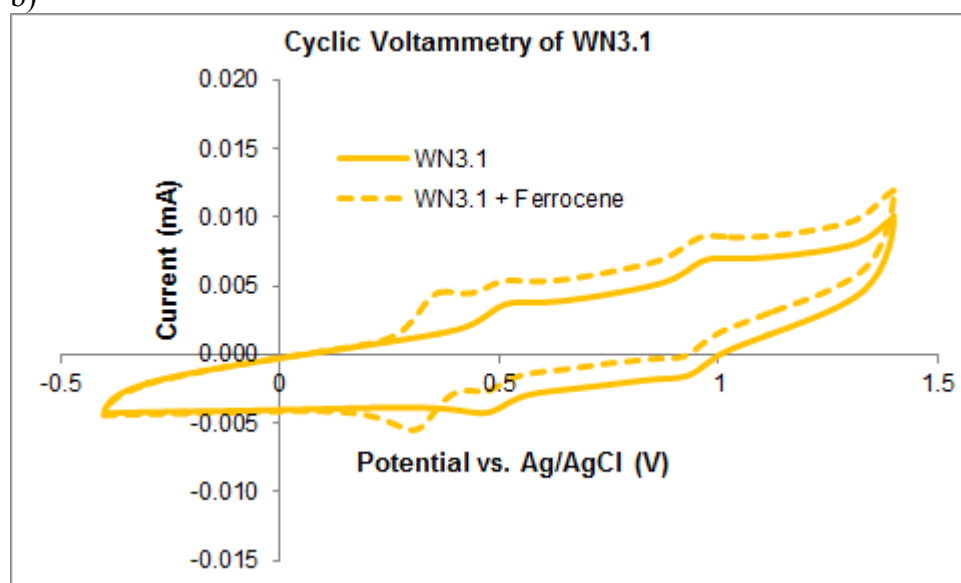


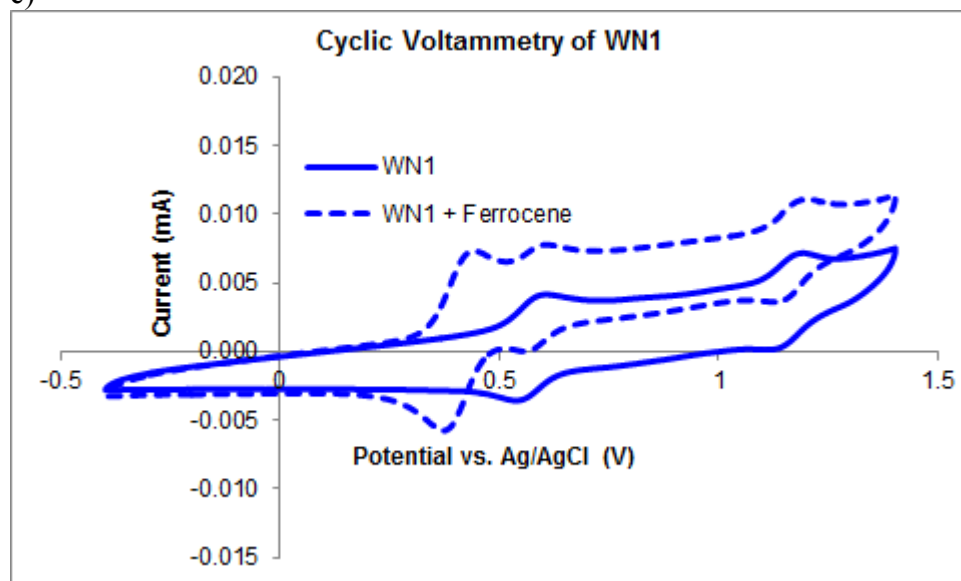
Figure SI6. Green arrow defining donor-to-acceptor perspective of a) D216, b) Y123, c) WN3.1, d) WN1, e) WN3, and f) C218, as depicted in Figures 6 and SI5.



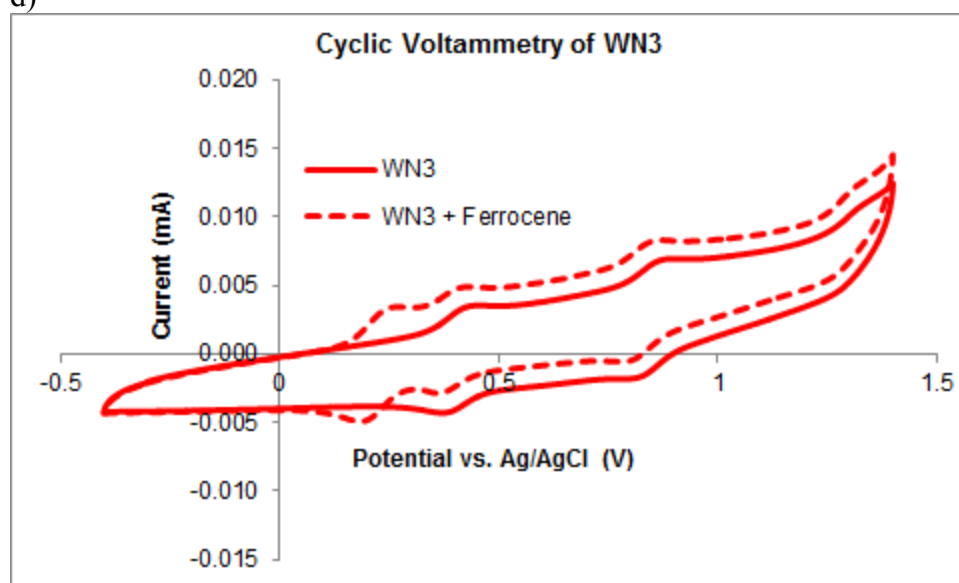
b)



c)



d)



e)

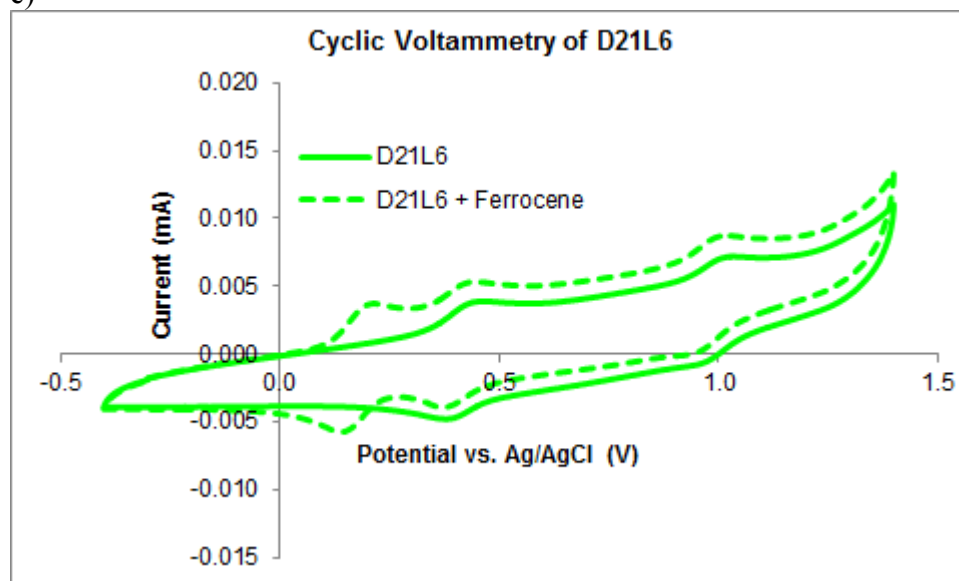
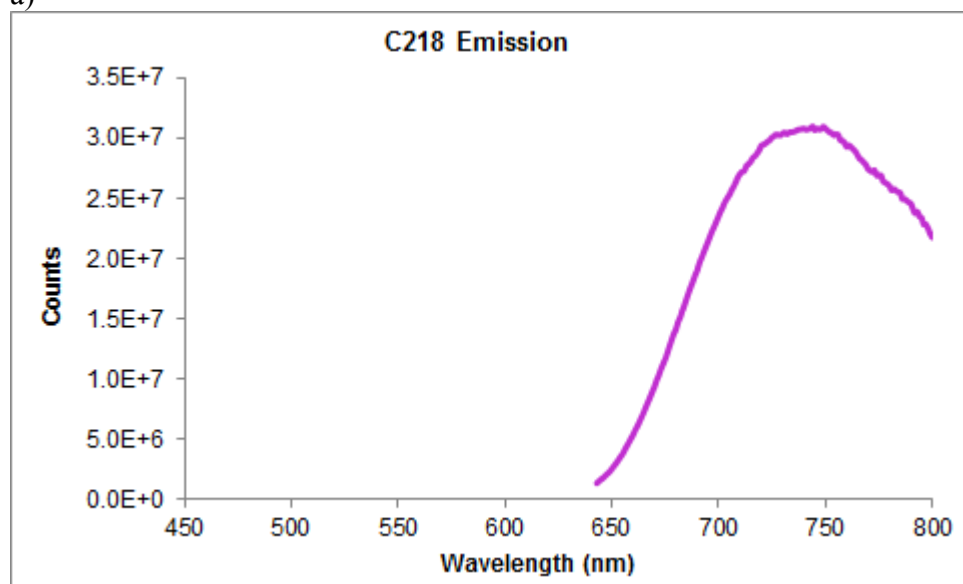
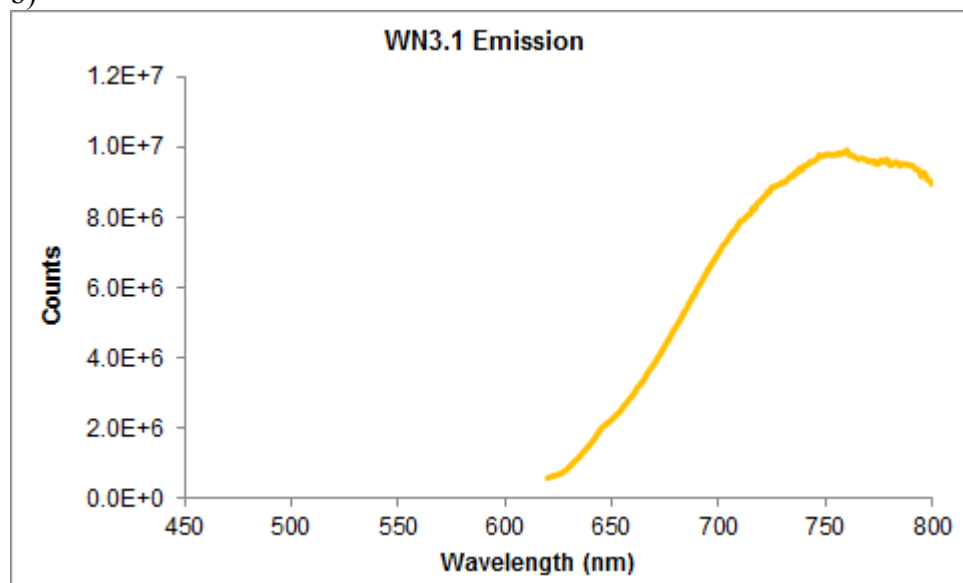


Figure SI7. Cyclic voltammetry curves of a) C218, b) WN3.1, c) WN1, d) WN3, and e) D21L6.

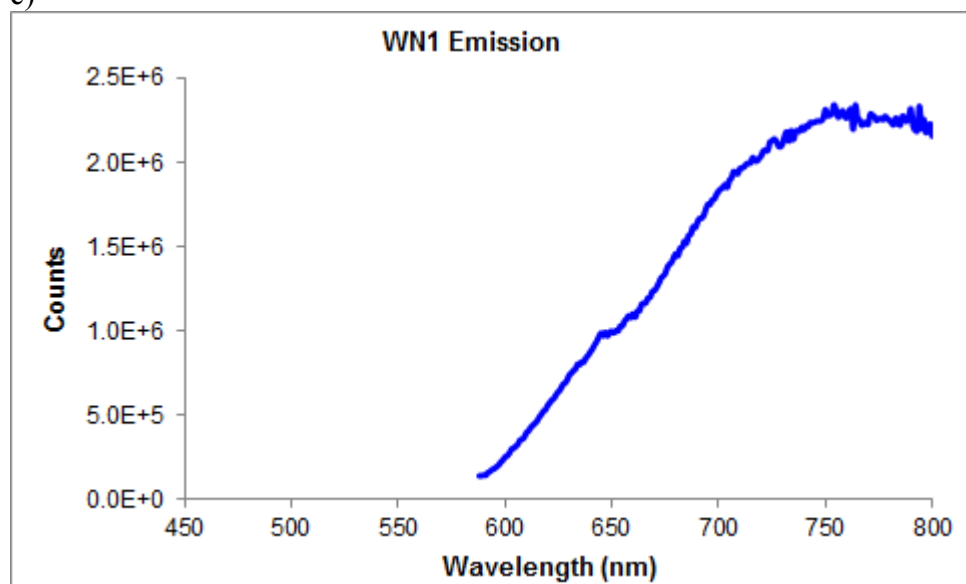
a)



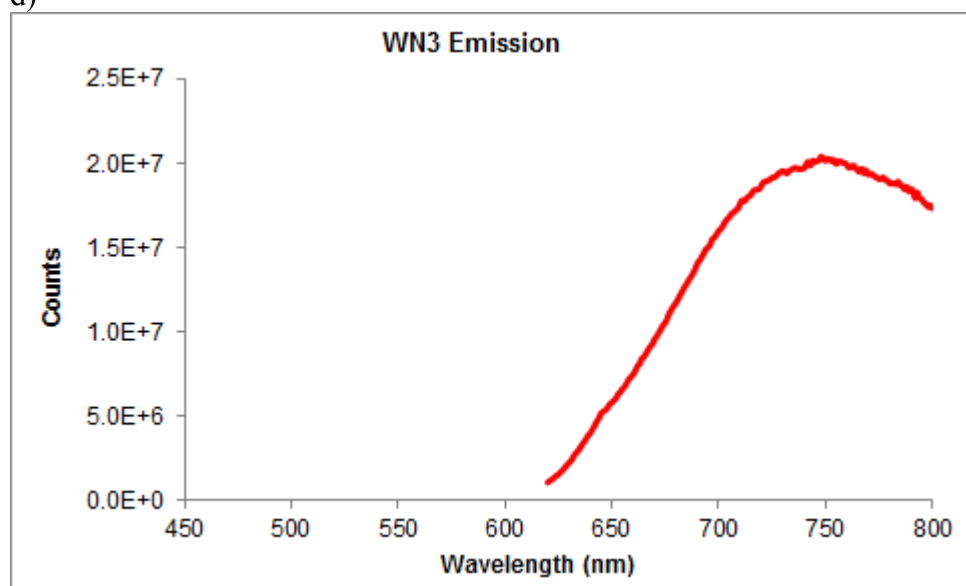
b)



c)



d)



e)

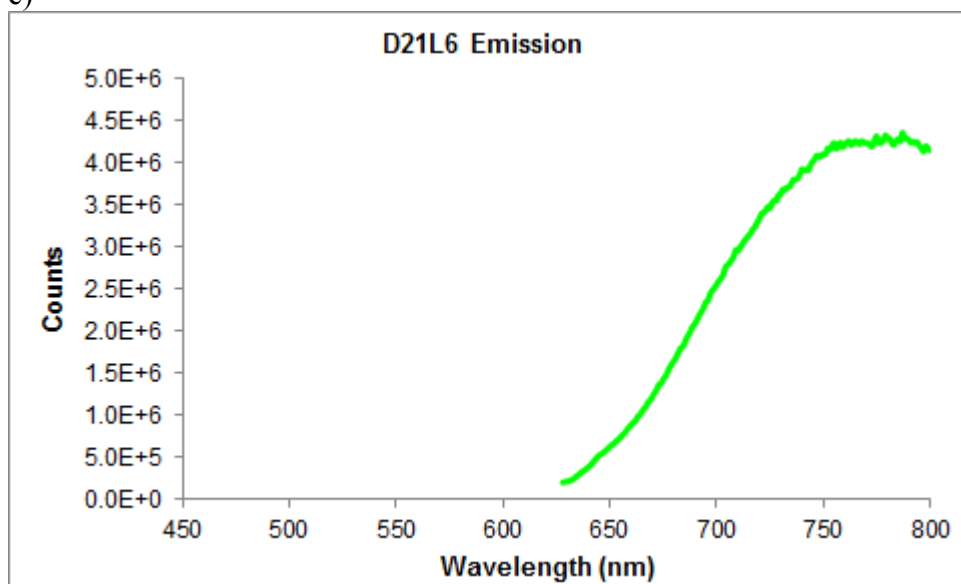


Figure SI8. Emission spectra of a) C218, b) WN3.1, c) WN1, d) WN3, and e) D21L6.

2. Analysis of Voc vs Capacitance

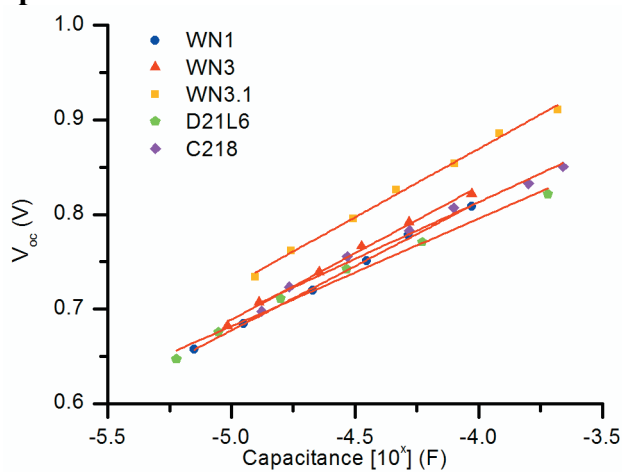


Figure SI9. Voc vs log(capacitance) dependence of dyes in this study determined by transient photovoltage/photocurrent measurements. Fits are linear and fit parameters are listed in Table SI1.

Table SI1. Fit parameters for Voc vs log(capacitance) as shown in Figure SI9.

Equation	Voc = a + b*log(capacitance)	
Dye	Fit Parameter	Value
WN1	a	1.35698
	b	0.13589
WN3	a	1.39069
	b	0.14033
WN3.1	a	1.44915
	b	0.14489
D21L6	a	1.2521
	b	0.11408
C218	a	1.29414
	b	0.12024

4. Raw data tables

Table SI2. Absorption data corresponding to Figure 3a in paper.

Wavelength (nm)	Dye				
	WN1	WN3	WN3.1	D21L6	C218
700	8	16	39	91	248
699	8	18	42	93	258
698	8	17	45	96	269
697	9	18	51	98	284
696	9	19	53	102	297
695	9	21	62	106	311
694	10	23	61	111	325
693	10	24	62	113	344
692	11	28	72	119	360
691	12	29	69	123	381
690	14	30	81	127	403
689	16	28	80	133	421
688	18	36	89	138	449
687	16	38	94	143	472
686	16	39	104	148	499
685	18	41	109	156	526
684	19	48	114	161	557
683	19	51	124	171	591
682	21	53	134	180	622
681	21	59	143	187	662
680	23	62	151	199	701
679	23	69	160	206	743
678	24	73	173	217	788
677	27	81	180	227	834
676	32	83	193	238	884
675	32	90	211	251	939
674	32	93	216	264	996
673	34	101	239	278	1060
672	38	109	249	293	1125
671	39	115	265	307	1194
670	42	127	283	325	1269
669	47	132	303	342	1349
668	48	142	318	361	1434
667	51	153	342	381	1524
666	55	171	371	402	1620
665	58	178	385	423	1720
664	60	191	415	446	1829
663	64	201	445	471	1944
662	69	217	466	498	2064
661	73	231	496	525	2196
660	78	248	535	554	2328
659	81	267	565	585	2477
658	92	290	597	618	2629
657	97	313	638	653	2793
656	100	331	681	687	2960

655	106	357	725	726	3142
654	114	382	769	769	3332
653	120	408	817	813	3533
652	127	440	869	856	3746
651	135	472	925	901	3970
650	144	503	983	951	4208
649	153	537	1044	1004	4456
648	164	579	1112	1058	4719
647	173	621	1174	1118	4998
646	184	668	1251	1178	5288
645	194	712	1328	1241	5595
644	208	766	1408	1308	5914
643	221	814	1495	1379	6247
642	237	872	1586	1454	6602
641	249	936	1682	1529	6965
640	265	1001	1787	1610	7352
639	283	1070	1893	1696	7757
638	301	1147	2003	1785	8175
637	319	1224	2122	1879	8616
636	339	1310	2248	1977	9070
635	359	1396	2381	2078	9546
634	381	1491	2517	2184	10038
633	405	1594	2667	2294	10557
632	430	1698	2820	2410	11094
631	455	1814	2985	2532	11651
630	484	1938	3160	2656	12226
629	515	2062	3339	2789	12830
628	547	2201	3529	2927	13452
627	578	2343	3729	3071	14094
626	614	2496	3936	3219	14759
625	651	2660	4155	3373	15443
624	692	2831	4394	3534	16150
623	733	3011	4642	3701	16880
622	777	3204	4890	3873	17625
621	824	3412	5159	4053	18396
620	873	3619	5440	4238	19179
619	925	3846	5731	4432	19990
618	979	4082	6043	4630	20821
617	1036	4332	6361	4836	21658
616	1098	4593	6690	5050	22533
615	1165	4873	7042	5270	23411
614	1232	5163	7397	5497	24306
613	1301	5468	7778	5730	25218
612	1379	5788	8172	5970	26142
611	1455	6122	8576	6219	27089
610	1536	6473	8998	6473	28047
609	1624	6837	9432	6735	29008
608	1716	7228	9892	7006	29986
607	1813	7626	10369	7283	30972
606	1913	8044	10862	7568	31973
605	2017	8481	11375	7861	32978
604	2128	8935	11909	8158	33981
603	2244	9410	12447	8466	34994
602	2367	9904	13020	8777	36011
601	2495	10417	13608	9099	37031
600	2627	10945	14208	9424	38049
599	2766	11495	14835	9756	39055
598	2912	12065	15472	10097	40072
597	3065	12664	16132	10443	41078
596	3222	13267	16805	10794	42082
595	3389	13897	17498	11153	43073
594	3561	14551	18210	11516	44053
593	3742	15220	18937	11890	45033
592	3930	15906	19685	12265	45987
591	4125	16612	20450	12642	46927
590	4330	17343	21220	13030	47860

589	4543	18089	22016	13421	48767
588	4765	18847	22828	13815	49663
587	4994	19637	23648	14215	50543
586	5231	20432	24484	14614	51395
585	5479	21245	25336	15020	52229
584	5737	22080	26194	15431	53046
583	6000	22918	27059	15840	53825
582	6277	23776	27952	16253	54589
581	6560	24646	28838	16663	55318
580	6855	25532	29735	17080	56030
579	7160	26418	30643	17496	56703
578	7471	27323	31539	17912	57345
577	7796	28230	32445	18330	57971
576	8129	29144	33354	18743	58556
575	8474	30050	34252	19153	59110
574	8829	30977	35165	19568	59642
573	9192	31897	36078	19980	60140
572	9563	32820	36978	20391	60608
571	9948	33735	37869	20796	61042
570	10342	34649	38764	21194	61444
569	10744	35555	39636	21591	61828
568	11160	36466	40516	21988	62173
567	11582	37365	41381	22378	62486
566	12013	38248	42235	22764	62770
565	12459	39119	43080	23144	63024
564	12908	39984	43887	23519	63249
563	13368	40831	44682	23883	63449
562	13832	41645	45461	24245	63613
561	14310	42465	46231	24602	63752
560	14788	43255	46976	24950	63865
559	15280	44031	47692	25291	63947
558	15777	44775	48389	25621	64001
557	16278	45495	49062	25943	64032
556	16784	46204	49696	26263	64033
555	17298	46881	50327	26566	64008
554	17817	47530	50916	26865	63960
553	18340	48153	51481	27155	63884
552	18868	48749	52013	27433	63782
551	19400	49313	52524	27704	63654
550	19933	49854	53005	27965	63505
549	20466	50366	53453	28211	63334
548	21007	50848	53875	28455	63134
547	21543	51301	54267	28685	62914
546	22085	51729	54624	28906	62665
545	22625	52125	54963	29116	62398
544	23163	52487	55261	29315	62109
543	23701	52823	55528	29502	61792
542	24234	53128	55780	29678	61453
541	24766	53403	55988	29846	61097
540	25293	53653	56175	30002	60718
539	25820	53872	56328	30147	60318
538	26340	54064	56459	30281	59891
537	26853	54226	56548	30403	59447
536	27358	54358	56627	30513	58986
535	27865	54473	56666	30617	58501
534	28358	54551	56682	30703	57998
533	28845	54603	56678	30780	57475
532	29324	54633	56639	30848	56934
531	29794	54641	56580	30903	56378
530	30257	54618	56490	30945	55800
529	30712	54563	56379	30978	55213
528	31150	54494	56241	31000	54602
527	31578	54399	56076	31007	53987
526	31993	54277	55890	31007	53351
525	32405	54131	55675	30994	52697
524	32800	53960	55449	30970	52032

523	33183	53763	55193	30935	51363
522	33555	53547	54916	30888	50671
521	33916	53307	54615	30834	49971
520	34259	53042	54291	30762	49264
519	34591	52755	53946	30686	48546
518	34907	52456	53580	30593	47828
517	35210	52120	53199	30493	47093
516	35504	51766	52791	30382	46350
515	35774	51395	52367	30260	45609
514	36032	51005	51928	30129	44858
513	36278	50592	51473	29988	44106
512	36503	50164	50996	29836	43347
511	36714	49722	50502	29675	42595
510	36911	49254	49998	29503	41835
509	37093	48765	49469	29321	41067
508	37258	48260	48936	29133	40308
507	37411	47749	48379	28934	39545
506	37544	47211	47828	28725	38784
505	37663	46667	47251	28513	38025
504	37765	46110	46662	28289	37273
503	37853	45533	46068	28059	36509
502	37924	44959	45469	27819	35766
501	37977	44362	44856	27570	35015
500	38019	43761	44241	27316	34277
499	38044	43153	43627	27052	33532
498	38051	42538	42990	26788	32798
497	38041	41912	42350	26513	32075
496	38020	41276	41721	26234	31349
495	37981	40645	41080	25948	30631
494	37930	40013	40439	25660	29927
493	37860	39369	39796	25362	29226
492	37779	38731	39143	25065	28536
491	37683	38084	38508	24760	27852
490	37572	37442	37860	24454	27181
489	37451	36800	37217	24143	26520
488	37311	36156	36580	23829	25864
487	37162	35512	35954	23514	25224
486	37003	34871	35315	23196	24594
485	36825	34233	34704	22876	23983
484	36644	33596	34077	22554	23381
483	36446	32964	33452	22232	22785
482	36241	32335	32836	21908	22204
481	36031	31708	32219	21588	21645
480	35805	31078	31608	21264	21091
479	35571	30469	31001	20940	20559
478	35331	29861	30401	20619	20034
477	35085	29251	29811	20300	19523
476	34830	28654	29221	19982	19031
475	34571	28062	28632	19668	18554
474	34301	27472	28058	19356	18087
473	34033	26893	27484	19050	17640
472	33757	26314	26916	18744	17211
471	33474	25751	26358	18448	16800
470	33191	25189	25794	18155	16395
469	32909	24641	25249	17867	16010
468	32624	24094	24716	17587	15641
467	32332	23555	24181	17312	15284
466	32041	23022	23659	17044	14941
465	31752	22507	23136	16784	14615
464	31458	21987	22628	16531	14305
463	31165	21485	22122	16288	14004
462	30872	20986	21627	16054	13716
461	30579	20496	21136	15830	13440
460	30290	20020	20650	15614	13185
459	29996	19543	20178	15408	12933
458	29706	19077	19711	15214	12692

457	29414	18618	19251	15027	12463
456	29125	18173	18795	14853	12245
455	28834	17731	18350	14689	12039
454	28546	17295	17913	14535	11839
453	28259	16863	17472	14393	11648
452	27976	16450	17052	14261	11470
451	27686	16037	16629	14140	11292
450	27405	15636	16215	14029	11130
449	27120	15244	15818	13928	10968
448	26836	14856	15420	13838	10814
447	26555	14472	15032	13761	10669
446	26272	14102	14659	13688	10526
445	25987	13732	14282	13628	10390
444	25709	13381	13921	13574	10260
443	25426	13031	13567	13533	10136
442	25144	12692	13213	13496	10011
441	24862	12354	12876	13470	9897
440	24580	12031	12551	13447	9782
439	24302	11720	12222	13432	9668
438	24021	11413	11913	13425	9568
437	23739	11112	11611	13423	9460
436	23459	10825	11316	13424	9353
435	23183	10550	11035	13432	9252
434	22902	10283	10767	13445	9159
433	22627	10028	10505	13461	9062
432	22351	9784	10263	13477	8965
431	22076	9556	10029	13502	8876
430	21807	9338	9814	13525	8786
429	21546	9140	9628	13552	8692
428	21284	8952	9443	13578	8605
427	21034	8784	9288	13602	8520
426	20791	8638	9142	13634	8433
425	20554	8507	9025	13666	8348
424	20328	8399	8932	13692	8266
423	20116	8308	8852	13722	8186
422	19919	8244	8812	13752	8106
421	19740	8203	8783	13782	8037
420	19580	8179	8781	13813	7959
419	19443	8188	8807	13839	7894
418	19329	8217	8863	13867	7826
417	19242	8284	8941	13893	7767
416	19184	8362	9053	13919	7709
415	19161	8467	9175	13946	7661
414	19171	8604	9345	13974	7614
413	19219	8760	9519	13999	7576
412	19307	8944	9736	14030	7543
411	19434	9146	9963	14058	7519
410	19604	9375	10225	14089	7509
409	19811	9628	10508	14125	7499
408	20065	9904	10801	14159	7499
407	20353	10199	11126	14200	7508
406	20683	10504	11470	14244	7524
405	21052	10835	11836	14290	7552
404	21448	11179	12211	14344	7583
403	21874	11539	12609	14400	7627
402	22324	11919	13000	14464	7679
401	22799	12309	13415	14534	7739
400	23279	12712	13837	14608	7803
399	23775	13112	14254	14689	7882
398	24263	13517	14679	14777	7962
397	24749	13927	15096	14866	8049
396	25219	14326	15511	14959	8149
395	25673	14722	15899	15066	8253
394	26101	15092	16285	15168	8364
393	26503	15459	16653	15282	8484
392	26871	15800	16987	15396	8607

391	27193	16119	17308	15512	8737
390	27482	16403	17590	15634	8867
389	27726	16671	17846	15757	9013
388	27920	16906	18068	15882	9157
387	28076	17106	18266	16005	9307
386	28186	17277	18435	16129	9454
385	28244	17416	18562	16253	9614
384	28263	17538	18668	16374	9764
383	28245	17620	18749	16492	9917
382	28187	17684	18806	16610	10066
381	28093	17725	18837	16721	10217
380	27967	17749	18855	16827	10361
379	27809	17750	18845	16925	10503
378	27628	17745	18832	17016	10633
377	27409	17722	18796	17098	10768
376	27178	17684	18754	17173	10883
375	26930	17643	18697	17235	10990
374	26657	17595	18629	17281	11090
373	26369	17537	18559	17322	11184
372	26068	17469	18483	17345	11267
371	25759	17411	18401	17354	11340
370	25431	17333	18309	17354	11403
369	25096	17270	18213	17333	11463
368	24753	17194	18127	17304	11504
367	24402	17116	18030	17256	11545
366	24043	17029	17926	17193	11566
365	23681	16946	17837	17121	11590
364	23302	16857	17704	17035	11601
363	22926	16766	17584	16938	11608
362	22541	16660	17465	16820	11612
361	22143	16563	17335	16697	11613
360	21739	16434	17185	16557	11600
359	21335	16299	17032	16412	11592
358	20920	16137	16851	16256	11580
357	20497	15969	16658	16085	11568
356	20073	15777	16455	15912	11556
355	19642	15557	16226	15731	11554
354	19203	15325	15983	15532	11558
353	18759	15083	15718	15339	11550
352	18320	14813	15451	15132	11561
351	17874	14538	15176	14924	11566
350	17433	14256	14887	14705	11578

Table SI3. J-V curve data corresponding to Figure 3c in the paper.

Voltage (V)	Current Density (mA cm ⁻²) of Dye					
	WN1	WN3	WN3.1	D21L6	C218	Y123
0	-8.38	-9.98	-9.58	-9.22	-10.30	-9.96
0.01	-8.36	-9.98	-9.58	-9.25	-10.25	-9.93
0.02	-8.36	-9.98	-9.60	-9.20	-10.27	-9.92
0.03	-8.39	-9.95	-9.48	-9.25	-10.28	-9.91
0.04	-8.37	-9.92	-9.53	-9.24	-10.30	-9.95
0.05	-8.38	-9.96	-9.59	-9.23	-10.22	-9.92
0.06	-8.36	-9.96	-9.53	-9.22	-10.27	-9.95
0.07	-8.36	-9.93	-9.56	-9.23	-10.21	-9.93
0.08	-8.30	-9.93	-9.56	-9.26	-10.24	-9.94
0.09	-8.31	-9.94	-9.57	-9.24	-10.25	-9.94
0.1	-8.33	-9.90	-9.56	-9.22	-10.17	-9.95
0.11	-8.31	-9.89	-9.54	-9.22	-10.26	-9.95
0.12	-8.30	-9.88	-9.54	-9.23	-10.22	-9.95
0.13	-8.33	-9.87	-9.52	-9.19	-10.22	-9.95
0.14	-8.24	-9.85	-9.53	-9.19	-10.24	-9.97
0.15	-8.30	-9.86	-9.51	-9.18	-10.21	-9.93
0.16	-8.34	-9.90	-9.50	-9.18	-10.21	-9.92
0.17	-8.31	-9.86	-9.54	-9.21	-10.19	-9.96

0.18	-8.30	-9.86	-9.52	-9.23	-10.24	-9.91
0.19	-8.28	-9.86	-9.50	-9.22	-10.19	-9.94
0.2	-8.34	-9.87	-9.47	-9.21	-10.20	-9.88
0.21	-8.29	-9.88	-9.48	-9.22	-10.22	-9.92
0.22	-8.31	-9.82	-9.51	-9.17	-10.20	-9.92
0.23	-8.30	-9.84	-9.51	-9.12	-10.18	-9.95
0.24	-8.30	-9.82	-9.49	-9.20	-10.17	-9.91
0.25	-8.32	-9.84	-9.52	-9.19	-10.17	-9.94
0.26	-8.32	-9.82	-9.48	-9.17	-10.20	-9.94
0.27	-8.28	-9.84	-9.55	-9.17	-10.21	-9.95
0.28	-8.31	-9.83	-9.53	-9.18	-10.19	-9.96
0.29	-8.30	-9.82	-9.52	-9.10	-10.21	-9.96
0.3	-8.30	-9.84	-9.47	-9.15	-10.17	-9.91
0.31	-8.30	-9.80	-9.51	-9.14	-10.18	-9.92
0.32	-8.29	-9.84	-9.52	-9.14	-10.20	-9.91
0.33	-8.30	-9.80	-9.48	-9.13	-10.20	-9.93
0.34	-8.30	-9.85	-9.49	-9.15	-10.20	-9.90
0.35	-8.30	-9.84	-9.47	-9.18	-10.22	-9.92
0.36	-8.29	-9.81	-9.48	-9.16	-10.20	-9.93
0.37	-8.23	-9.78	-9.50	-9.14	-10.20	-9.91
0.38	-8.26	-9.81	-9.45	-9.10	-10.16	-9.92
0.39	-8.24	-9.79	-9.50	-9.13	-10.16	-9.93
0.4	-8.24	-9.79	-9.45	-9.13	-10.18	-9.93
0.41	-8.23	-9.80	-9.51	-9.12	-10.18	-9.93
0.42	-8.16	-9.74	-9.47	-9.14	-10.14	-9.91
0.43	-8.23	-9.80	-9.52	-9.10	-10.17	-9.90
0.44	-8.23	-9.75	-9.42	-9.12	-10.14	-9.92
0.45	-8.23	-9.75	-9.47	-9.12	-10.19	-9.94
0.46	-8.25	-9.75	-9.41	-9.11	-10.15	-9.94
0.47	-8.24	-9.73	-9.46	-9.06	-10.13	-9.92
0.48	-8.21	-9.71	-9.49	-9.08	-10.16	-9.84
0.49	-8.21	-9.71	-9.49	-9.05	-10.15	-9.93
0.5	-8.18	-9.67	-9.46	-9.02	-10.18	-9.90
0.51	-8.21	-9.72	-9.46	-9.01	-10.16	-9.91
0.52	-8.20	-9.69	-9.45	-8.97	-10.10	-9.90
0.53	-8.15	-9.68	-9.44	-8.99	-10.12	-9.87
0.54	-8.15	-9.68	-9.48	-8.95	-10.08	-9.87
0.55	-8.10	-9.60	-9.46	-8.91	-10.11	-9.88
0.56	-8.10	-9.63	-9.47	-8.88	-10.07	-9.87
0.57	-8.08	-9.59	-9.45	-8.80	-10.04	-9.87
0.58	-8.05	-9.54	-9.42	-8.77	-10.03	-9.84
0.59	-7.98	-9.50	-9.38	-8.71	-9.96	-9.81
0.6	-7.93	-9.42	-9.42	-8.62	-9.90	-9.82
0.61	-7.87	-9.34	-9.41	-8.52	-9.87	-9.82
0.62	-7.79	-9.27	-9.38	-8.39	-9.79	-9.78
0.63	-7.71	-9.17	-9.32	-8.28	-9.71	-9.73
0.64	-7.58	-9.02	-9.32	-8.14	-9.58	-9.69
0.65	-7.46	-8.87	-9.26	-7.96	-9.52	-9.61
0.66	-7.30	-8.69	-9.23	-7.75	-9.39	-9.58
0.67	-7.14	-8.46	-9.17	-7.54	-9.25	-9.50
0.68	-6.94	-8.21	-9.12	-7.29	-9.05	-9.41
0.69	-6.68	-7.96	-9.00	-6.96	-8.84	-9.31
0.7	-6.42	-7.67	-8.90	-6.59	-8.61	-9.23
0.71	-6.12	-7.33	-8.72	-6.22	-8.33	-9.10
0.72	-5.77	-6.98	-8.61	-5.76	-8.05	-8.94
0.73	-5.40	-6.57	-8.42	-5.24	-7.70	-8.74
0.74	-4.93	-6.16	-8.22	-4.66	-7.32	-8.53
0.75	-4.45	-5.69	-7.96	-4.04	-6.83	-8.29
0.76	-3.91	-5.16	-7.65	-3.30	-6.36	-8.03
0.77	-3.34	-4.57	-7.31	-2.50	-5.77	-7.75
0.78	-2.68	-3.97	-6.91	-1.60	-5.11	-7.38
0.79	-1.97	-3.29	-6.49	-0.60	-4.37	-6.95
0.8	-1.24	-2.55	-5.95	0.50	-3.56	-6.51
0.81	-0.35	-1.78	-5.37	1.74	-2.66	-5.98
0.82	0.58	-0.94	-4.67	3.08	-1.66	-5.41
0.83	1.54	-0.02	-3.92	4.55	-0.49	-4.74

0.84	2.55	0.98	-3.11	6.15	0.80	-4.00
0.85	3.62	2.02	-2.22	7.88	2.17	-3.18
0.86	4.78	3.13	-1.23	9.75	3.66	-2.26
0.87	6.06	4.29	-0.13	11.73	5.32	-1.25
0.88	7.36	5.59	1.16		7.10	-0.15
0.89	8.73	6.91	2.47		9.00	1.05
0.9	10.16	8.30	3.86		11.03	2.37
0.91	11.66	9.76	5.43		13.20	3.80
0.92	13.24	11.29	7.04		15.49	5.32
0.93	14.87	12.89	8.75		17.91	6.96
0.94	16.58	14.56	10.58		20.46	8.70
0.95	18.35	16.31	12.50		23.13	10.55
0.96	20.20	18.12	14.53		25.93	12.50
0.97	22.10	20.00	16.66		28.84	
0.98	24.04	21.94	18.88		31.85	
0.99	26.04	23.94	21.18		34.96	
1	28.09	25.97	23.53		38.14	

Table SI4. EQE data corresponding to Figure 3b in the paper

Wavelength (nm)	Dye				
	WN1	WN3	WN3.1	D21L6	C218
380	54.0	39.5	31.2	50.0	25.6
390	47.9	34.1	35.4	41.3	28.2
400	48.1	38.2	39.5	40.8	32.0
410	57.6	51.1	51.8	50.2	44.8
420	69.2	63.2	67.0	63.2	55.4
430	69.6	67.4	72.0	68.2	64.9
440	71.6	66.5	71.1	69.8	65.9
450	71.4	68.9	74.7	71.7	70.0
460	71.9	69.2	73.0	71.3	70.1
470	71.3	67.5	70.2	69.6	69.0
480	71.6	68.9	69.4	70.8	69.1
490	69.2	66.0	69.5	67.7	67.0
500	68.5	65.5	69.2	65.2	66.4
510	66.7	64.3	70.8	63.7	67.1
520	64.1	63.2	66.8	61.8	64.4
530	62.3	61.3	65.4	60.4	63.3
540	60.7	61.1	68.7	59.7	63.9
550	58.3	61.4	67.8	58.0	64.6
560	58.4	62.2	70.0	59.6	63.9
570	50.8	57.0	63.8	54.5	61.9
580	43.5	50.9	57.2	47.5	57.9
590	39.4	47.4	53.7	43.5	59.1
600	31.5	40.6	46.4	38.3	50.2
610	21.4	29.4	31.4	29.2	44.3
620	16.6	22.5	25.6	21.9	40.0
630	13.4	18.1	20.7	18.6	34.2
640	8.9	12.3	10.9	14.2	24.6
650	4.4	6.6	4.3	9.1	16.8
660	2.4	2.7	4.2	5.5	12.9
670	1.5	1.5	1.8	3.7	8.3
680	0.7	1.1	0.0	1.2	4.1
690	1.2	1.1	0.0	1.1	1.2
700	1.5	2.8	0.4	1.7	0.0
710	1.8	2.3	0.7	1.9	0.0
720	2.3	2.6	0.3	2.3	1.6
730	2.0	2.8	2.6	2.1	1.0
740	2.9	2.5	1.6	2.4	3.3
750	3.1	3.5	2.1	3.1	1.9

Table SI5. Recombination lifetime vs capacitance data corresponding to Figure 5b in main text.

WN1	Capacitance (F)	9.39E-05	5.19E-05	3.52E-05	2.14E-05	1.12E-05	7.07E-06	
	Recombination Lifetime (s)	7.80E-04	1.29E-03	1.95E-03	3.15E-03	5.14E-03	7.84E-03	
WN3	Capacitance (F)	9.37E-05	5.24E-05	3.36E-05	2.27E-05	1.29E-05	9.65E-06	
	Recombination Lifetime (s)	7.25E-04	1.25E-03	2.04E-03	3.29E-03	5.76E-03	8.67E-03	
WN3.1	Capacitance (F)	2.08E-04	1.21E-04	7.99E-05	4.63E-05	3.11E-05	1.75E-05	1.25E-05
	Recombination Lifetime (s)	6.56E-04	1.08E-03	1.93E-03	3.48E-03	6.12E-03	1.12E-02	1.68E-02
D21L6	Capacitance (F)	1.91E-04	5.92E-05	2.92E-05	1.59E-05	8.88E-06	6.00E-06	
	Recombination Lifetime (s)	5.61E-04	1.15E-03	1.87E-03	3.36E-03	6.20E-03	1.01E-02	
C218	Capacitance (F)	2.19E-04	1.59E-04	7.91E-05	5.24E-05	2.94E-05	1.72E-05	1.32E-05
	Recombination Lifetime (s)	5.61E-04	7.31E-04	1.08E-03	1.88E-03	3.31E-03	6.05E-03	9.18E-03
Y123	Capacitance (F)	9.42E-05	5.61E-05	3.67E-05	2.11E-05	1.37E-05	1.03E-05	
	Recombination Lifetime (s)	9.66E-04	0.00156	0.00277	0.005	0.00928	0.01479	

Table SI6. Emission data of C218 corresponding to Figure SI8a.

Wavelength (nm)	Counts
643	1382538
644	1548633
645	1710651
646	1825143
647	2011512
648	2191193
649	2352882
650	2573926
651	2799721
652	3041877
653	3284265
654	3559234
655	3789041
656	4130410
657	4448570
658	4768460
659	5094410
660	5399401
661	5810012
662	6136149
663	6513965
664	6895972

665	7292998
666	7721082
667	8127256
668	8544960
669	8986560
670	9396211
671	9924611
672	10332354
673	10828550
674	11281484
675	11682526
676	12197680
677	12754924
678	13264260
679	13770760
680	14144954
681	14763854
682	15139228
683	15684168
684	16137955
685	16683644
686	17198564
687	17685977
688	18162599
689	18643227
690	19057771
691	19649987
692	20082620
693	20541651
694	20979554
695	21423011
696	21882853
697	22323496
698	22698125
699	23114149
700	23516631
701	23985886
702	24328159
703	24747045
704	25038555
705	25305073

706	25697766
707	25986425
708	26358851
709	26770099
710	27049652
711	27254600
712	27287704
713	27705299
714	27866850
715	28054825
716	28399735
717	28515323
718	28771181
719	29028911
720	29439688
721	29482772
722	29603272
723	29750267
724	29864398
725	30084373
726	30189710
727	30350925
728	30272813
729	30264786
730	30426094
731	30501721
732	30357111
733	30512168
734	30516959
735	30553419
736	30610642
737	30725599
738	30751233
739	30784402
740	30847051
741	30714290
742	30789881
743	30818981
744	31002952
745	30704571
746	30831450

747	30728913
748	30785766
749	30981240
750	30832745
751	30668875
752	30527577
753	30455147
754	30274912
755	30353352
756	30297491
757	29861320
758	29839112
759	29622039
760	29304473
761	29430286
762	29287898
763	29125664
764	28944960
765	28633617
766	28328275
767	28212950
768	27985328
769	27810104
770	27461463
771	27334560
772	27232681
773	27362476
774	26934967
775	26941898
776	26960608
777	26452397
778	26352429
779	26210460
780	26052731
781	25701473
782	25816778
783	25657848
784	25560661
785	25502156
786	24980331
787	24991065

788	24847785
789	24697171
790	24601802
791	24135098
792	23799085
793	23951328
794	23522799
795	23422628
796	22872544
797	22876838
798	22555409
799	22122667
800	21799395

Table SI7. Emission data of WN3.1 corresponding to Figure SI8b.

Wavelength (nm)	Counts
620	591279.02
621	623558.7
622	642027.86
623	659976.31
624	680763.83
625	692873.72
626	722296.66
627	753761.34
628	795993.43
629	843524.58
630	902731.45
631	961400
632	1029662
633	1084856.5
634	1141857.3
635	1207654.6
636	1276462.3
637	1356104.1
638	1427501
639	1490053.8
640	1563659.3
641	1643276.9
642	1718118.5
643	1823697.6

644	1904313.4
645	2007301.4
646	2055654.2
647	2106810.7
648	2165436.7
649	2211886.9
650	2255834.7
651	2314366.2
652	2389671.6
653	2430845.3
654	2493495.7
655	2590117
656	2672751.4
657	2723340.8
658	2817589.5
659	2883088.6
660	2961311.7
661	3055143
662	3176171.9
663	3224883.5
664	3308810.5
665	3391959.9
666	3502988.2
667	3611738.2
668	3694400.9
669	3767141.8
670	3858850.3
671	3950164.1
672	4062716.2
673	4149920.7
674	4268088.1
675	4373061.3
676	4478059.2
677	4571066.4
678	4687039.3
679	4803480.2
680	4888630.3
681	4995740
682	5091241.8
683	5194212
684	5343006.2

685	5400135.1
686	5545510.1
687	5637983.7
688	5758660.5
689	5849994.8
690	5981249.4
691	6074417.9
692	6177756
693	6295173.4
694	6396203.9
695	6516871.1
696	6608743.6
697	6711760.9
698	6801914.9
699	6910326.9
700	6984728.8
701	7114283.9
702	7206456.3
703	7273022.3
704	7360458.6
705	7442856.5
706	7539272.6
707	7623400.7
708	7673920.2
709	7779188.3
710	7898602.3
711	7920861.3
712	7959316.8
713	8030373.1
714	8082963.3
715	8117435.2
716	8282079.8
717	8250270
718	8402272.1
719	8446866.6
720	8514301.5
721	8577220
722	8625819.8
723	8747267.1
724	8740868.2
725	8882681.1

726	8878083.4
727	8915849.4
728	8939762.8
729	8966654.8
730	9022575.9
731	9009324.5
732	9069084.3
733	9141914.3
734	9200217.1
735	9182261.1
736	9304141
737	9282167.7
738	9414562.3
739	9353026.4
740	9469469
741	9492324.4
742	9509452.3
743	9607116.5
744	9581892.4
745	9633818.5
746	9676340.2
747	9781500.5
748	9771860.3
749	9751325.4
750	9802176.9
751	9799447.4
752	9810347.4
753	9783346
754	9799344.2
755	9792636
756	9838482.9
757	9804750.7
758	9859264
759	9851952.4
760	9923991.9
761	9792700.1
762	9776726
763	9763752.8
764	9715579.4
765	9685306.9
766	9686593.8

767	9697368.3
768	9685886.3
769	9642636.5
770	9607794.1
771	9629583.9
772	9583540.4
773	9618268.7
774	9525452.8
775	9552516.7
776	9647467
777	9586520.4
778	9625351.2
779	9656550.4
780	9502812.4
781	9508287.2
782	9556674.4
783	9596357.9
784	9554035.8
785	9475619.9
786	9537024.3
787	9516365.5
788	9533955.6
789	9501068.1
790	9494739.5
791	9473774.8
792	9389471.1
793	9378055.5
794	9323866.3
795	9177582
796	9292546.2
797	9191915.2
798	9077114.8
799	9044381.9
800	8959226.6

Table SI8. Emission data of WN1 corresponding to Figure SI8c.

Wavelength (nm)	Counts
580	355883.85
581	330801.39
582	299194.08

583	263290.55
584	230941.16
585	202846.21
586	173218.27
587	153145.13
588	143153.25
589	144481.33
590	146657.07
591	145769.79
592	161953.43
593	168468.04
594	180667.38
595	185512.38
596	196216.86
597	206276.77
598	223407.6
599	235653.35
600	254232.94
601	260732.08
602	276570.46
603	299252.72
604	307040.57
605	316933.45
606	329605.54
607	353830.56
608	360243.65
609	370058.11
610	399118.48
611	408146.23
612	428391.64
613	441203.34
614	454236.37
615	466852.01
616	490251.7
617	505687.95
618	525644.75
619	535776.19
620	558856.13
621	577134.58
622	593660.59
623	603113.38

624	625515.46
625	640293.11
626	656133.13
627	682375.32
628	692408.07
629	707456.49
630	738472.74
631	750431.13
632	766086.13
633	775756.42
634	805434.39
635	801490.05
636	820735.77
637	818033.53
638	843917.37
639	857675.4
640	878805.71
641	895887.71
642	920889.4
643	940766.87
644	967933.8
645	989832.53
646	973053.02
647	993194.89
648	972270.54
649	992700.02
650	1000514.5
651	990973.4
652	1004585.3
653	1002068.6
654	1031066.9
655	1031850.4
656	1061212.6
657	1074088.7
658	1093250.1
659	1082021.6
660	1104572
661	1083205.1
662	1120105.9
663	1123329.2
664	1161820.5

665	1164215.1
666	1170608.7
667	1199024.5
668	1202464.7
669	1237051.8
670	1241185.7
671	1260119.4
672	1283944
673	1314110.3
674	1326662.5
675	1342327.1
676	1378151
677	1397375
678	1408589.6
679	1437469.8
680	1460821.5
681	1447737.4
682	1492642.2
683	1496528
684	1534291.7
685	1521905.1
686	1569475.6
687	1575429.6
688	1619795.8
689	1611630.9
690	1643675.1
691	1668505.6
692	1669934
693	1686871.6
694	1723272.9
695	1752831.4
696	1752664
697	1778717.5
698	1783913.9
699	1810831.4
700	1830108
701	1844749.9
702	1851093.6
703	1869392.4
704	1852198.3
705	1893799.3

706	1908423
707	1946630.5
708	1938194.3
709	1933800
710	1964844.9
711	1968534.5
712	1975371.9
713	1991484.3
714	1996033.1
715	1998648.9
716	2031101.2
717	2013613.1
718	2008791.5
719	2024904.9
720	2041589.5
721	2070934
722	2071512.8
723	2071269.6
724	2119840
725	2129718.1
726	2139454.2
727	2127566.3
728	2098415.1
729	2093306.6
730	2115403.1
731	2160301.1
732	2182018.8
733	2127353.6
734	2190418.5
735	2136272.3
736	2182524
737	2190768.5
738	2185999.3
739	2209731.2
740	2194768.1
741	2218114.2
742	2212196.8
743	2239160
744	2235283.7
745	2238925.7
746	2246180.1

747	2246707.8
748	2247812
749	2262830.6
750	2313913.2
751	2278736.3
752	2281653.8
753	2288289
754	2341868.2
755	2310768.1
756	2267704.3
757	2285444.1
758	2308065.1
759	2278172.7
760	2265204.9
761	2299367.7
762	2317287.8
763	2198278.6
764	2340815.7
765	2269751.4
766	2252679.9
767	2221231.5
768	2232481.8
769	2238695.1
770	2226880.7
771	2287585.3
772	2280724.5
773	2271165.2
774	2249214
775	2260088.8
776	2262590.6
777	2255168
778	2274797.9
779	2259916.2
780	2251484.9
781	2236647.5
782	2224291.3
783	2264304.2
784	2240169.3
785	2222083.5
786	2273969.1
787	2265183.3

788	2245131
789	2268008.5
790	2319384.2
791	2219212.6
792	2193144.5
793	2187353.1
794	2334026.1
795	2201744.8
796	2256942
797	2179746.9
798	2199514.6
799	2230210.5
800	2157072.6

Table SI9. Emission data of WN3 corresponding to Figure SI8d.

Wavelength (nm)	Counts
620	1092529.4
621	1200668
622	1269148.8
623	1386604.9
624	1492050.1
625	1572357
626	1708303.5
627	1818728.3
628	1980258.3
629	2124452.6
630	2270298.7
631	2387385.6
632	2619464.8
633	2802942.9
634	2936824.9
635	3128212.9
636	3324218.7
637	3497103
638	3685398.1
639	3892650.5
640	4036172.9
641	4258751.1
642	4461420.4
643	4719012.9

644	4912545.4
645	5206067.7
646	5301130.4
647	5382434.7
648	5523259.4
649	5726439.7
650	5846699.2
651	5956873.2
652	6104525.9
653	6327220
654	6462677.9
655	6651739.2
656	6771743.8
657	6992690.6
658	7207648.5
659	7348691
660	7510660.6
661	7705987.4
662	7996608.9
663	8119837.7
664	8435269.2
665	8531629.2
666	8739614.5
667	8970280.6
668	9150940
669	9291017.6
670	9598720.7
671	9747486.9
672	9969071.2
673	10182876
674	10418055
675	10562847
676	10836403
677	11150253
678	11368277
679	11571181
680	11739384
681	11952521
682	12203089
683	12420794
684	12664373

685	12873662
686	13087406
687	13278440
688	13498908
689	13747349
690	14072576
691	14234301
692	14452855
693	14671223
694	14907395
695	15024861
696	15181638
697	15515714
698	15618085
699	15807161
700	15991163
701	16122501
702	16307208
703	16543904
704	16709773
705	16823925
706	17030656
707	17094537
708	17229263
709	17337964
710	17606580
711	17830745
712	17761835
713	17906672
714	18053671
715	18126537
716	18358576
717	18447929
718	18454510
719	18490179
720	18699749
721	18909806
722	18934936
723	19003664
724	19044236
725	19175405

726	19180047
727	19268178
728	19418963
729	19486598
730	19562313
731	19497857
732	19422457
733	19569228
734	19629034
735	19718888
736	19747633
737	19714119
738	19654565
739	19726906
740	19707207
741	19953324
742	20112998
743	19884919
744	20172169
745	20094109
746	20148365
747	20206760
748	20414548
749	20295033
750	20156634
751	20290045
752	20278366
753	20130846
754	20224863
755	19974862
756	20118377
757	20142341
758	20058125
759	20036690
760	19931456
761	19749117
762	19777677
763	19895159
764	19753193
765	19611731
766	19503955

767	19705242
768	19430862
769	19610819
770	19347168
771	19383085
772	19378737
773	19223902
774	19180089
775	19080290
776	19088666
777	19192856
778	19005765
779	19012124
780	18824522
781	18830006
782	18857253
783	18761768
784	18934180
785	18704680
786	18688716
787	18483052
788	18640688
789	18370022
790	18495958
791	18370557
792	17946312
793	18303047
794	17939038
795	17915458
796	17674948
797	17621519
798	17429378
799	17532074
800	17337919

Table SI10. Emission data of D21L6 corresponding to Figure SI8e.

Wavelength (nm)	Counts
620	287721.68
621	289283.96
622	280356.44

623	267284.21
624	254867.12
625	234158.39
626	227939.07
627	213573.85
628	208326.81
629	212963.91
630	220840.81
631	223519.57
632	236784.64
633	250681.5
634	274354.23
635	290703.22
636	310968.32
637	337201.97
638	347473.86
639	368293
640	391500.63
641	411992.38
642	440858.16
643	473113.24
644	504086.25
645	526575.28
646	544529.83
647	561542.9
648	584415.98
649	604424.02
650	630091.12
651	653970.9
652	669802.78
653	699773.48
654	715130.38
655	744658.57
656	770438.71
657	793189.83
658	829863.3
659	861094.5
660	887706.92
661	917243.09
662	937150.08
663	986689.28

664	1006185.8
665	1043716.2
666	1080852.9
667	1109718.5
668	1163433.7
669	1184393.6
670	1226463
671	1271211.1
672	1308113
673	1368087.4
674	1379194.9
675	1431283.3
676	1461258.7
677	1515759.1
678	1570125.4
679	1611940.2
680	1646417.3
681	1690620.6
682	1741589.1
683	1795834.5
684	1812613.3
685	1855444.1
686	1924502.4
687	1959934.8
688	2013790.7
689	2065069.8
690	2092884.9
691	2146037.9
692	2195159.5
693	2236988.8
694	2284649.2
695	2346518.5
696	2366757.5
697	2442843.3
698	2483661.1
699	2515397.5
700	2552683.1
701	2597196.5
702	2624824.4
703	2665202.7
704	2747748.7

705	2785411.4
706	2807968.7
707	2847443.7
708	2884913.6
709	2966980
710	2949838.6
711	2998163.3
712	3027337.3
713	3070929.3
714	3103762.8
715	3134963.3
716	3165253.3
717	3212878.7
718	3235794.8
719	3295048.5
720	3329874.5
721	3394081.8
722	3407843
723	3431345.3
724	3475697.6
725	3460529
726	3522654.4
727	3552286.1
728	3545533.5
729	3621249.1
730	3621949.3
731	3684194
732	3677051.7
733	3707582.8
734	3712344.4
735	3751150.2
736	3799228.3
737	3799878.5
738	3814026.9
739	3862330.6
740	3923087.6
741	3900326.9
742	3922146.6
743	3909199.5
744	3975067.5
745	4011817.1

746	4047526.3
747	4086901.9
748	4065300.1
749	4091722.1
750	4094725.2
751	4099105.6
752	4168213.5
753	4149809.4
754	4198989
755	4234680.7
756	4165236.2
757	4192113.9
758	4238936.9
759	4180970.4
760	4220281.1
761	4239317.8
762	4257562.1
763	4207891
764	4235301.6
765	4257682.2
766	4238618
767	4220160.5
768	4255126.5
769	4240605.8
770	4227387
771	4233025.3
772	4201081.6
773	4195130.4
774	4273499
775	4312670.1
776	4232417.1
777	4236251.5
778	4259721
779	4326468
780	4282432.7
781	4288023.5
782	4229824.5
783	4210972
784	4256796.3
785	4280956.6
786	4251180.9

787	4354928.1
788	4289788.2
789	4293067.9
790	4266454.7
791	4233428.1
792	4252223.3
793	4228559.4
794	4242286.7
795	4192668.3
796	4166590.7
797	4131126.7
798	4195747.6
799	4167793.4
800	4144599.6

Table SI11. Optimized geometry coordinates C218 corresponding to Figure SI4a.

N	3.83307600	-0.33697600	-0.19419300
C	2.43255600	-0.42498200	-0.15805600
C	4.64133800	-1.50738900	-0.32659700
C	4.48727000	0.92571000	-0.05802400
C	5.71267700	-1.73160300	0.54296600
C	6.53119500	-2.85411400	0.40514700
C	6.27080400	-3.78851900	-0.60480800
C	5.19188800	-3.57272000	-1.47660400
C	4.39631000	-2.44304300	-1.34655000
C	5.48563600	1.30994100	-0.95795100
C	6.15351700	2.52837400	-0.81769400
C	5.81085000	3.39551000	0.22694800
C	4.80493100	3.01793300	1.13027400
C	4.16122300	1.79608600	0.99636600
O	6.99755600	-4.92204500	-0.82406400
O	6.38693200	4.61075400	0.45447700
C	8.10987700	-5.19458500	0.02704800
C	8.74441900	-6.50300600	-0.42442100
C	9.96439400	-6.87668300	0.42712800
C	10.62462600	-8.19423500	-0.00004900
C	11.84886100	-8.56206500	0.84766600
C	12.50570200	-9.87873200	0.42069000
C	7.42086600	5.05830700	-0.42117100
C	7.87608000	6.42831900	0.06245800
C	8.99750900	7.01884800	-0.80198500
C	9.45666300	8.40241900	-0.32405800
C	10.58036400	9.00353900	-1.17805700
C	11.03127200	10.38543300	-0.69429000

C	1.62715400	0.65525500	-0.57583800
C	0.24450600	0.57127800	-0.53146800
C	-0.41308900	-0.58882400	-0.07399600
C	0.39850400	-1.66627800	0.33116000
C	1.78316100	-1.59129600	0.29493600
C	-1.86959800	-0.64836500	-0.02512100
S	-2.71603400	-2.19985800	-0.09379600
C	-4.24617500	-1.39781500	0.01595900
C	-4.11719100	-0.01560300	0.09812600
C	-2.77000700	0.40475200	0.06379900
C	-5.63077100	-1.74403800	0.01619700
C	-6.39507700	-0.57315800	0.09420500
C	-5.49054400	0.66204500	0.16188900
S	-6.57680900	-3.18253300	-0.02684300
C	-8.06617800	-2.21628600	0.07938100
C	-7.76313800	-0.84712200	0.14271300
C	-9.38776700	-2.72846200	0.10202800
C	-9.86415100	-4.01798000	0.05005400
C	-5.73458100	1.39463700	1.51587200
C	-4.87137200	2.63171600	1.79746300
C	-5.21438800	3.28990100	3.14206000
C	-4.35631500	4.52342500	3.45063200
C	-4.70356300	5.19398600	4.78616400
C	-3.83979200	6.42311200	5.08676500
C	-5.65335800	1.59116700	-1.07879900
C	-6.99716300	2.31744800	-1.22464300
C	-7.04365200	3.21178600	-2.47230500
C	-8.38277700	3.93780200	-2.65330700
C	-8.42779700	4.83881600	-3.89428200
C	-9.76920300	5.55749400	-4.07086100
C	-11.31045400	-4.31349700	0.09307700
O	-11.79577400	-5.42591200	0.05079900
O	-12.08178400	-3.19188100	0.18787800
C	-9.01061200	-5.15576300	-0.04761600
N	-8.28776300	-6.06612100	-0.12722300
H	5.91502000	-1.01614800	1.33412700
H	7.35543000	-2.99286100	1.09485600
H	5.00581700	-4.29948600	-2.26120800
H	3.57333200	-2.27892500	-2.03551300
H	5.74910000	0.64522700	-1.77499300
H	6.92526500	2.79212400	-1.53168700
H	4.55694800	3.69474900	1.94199000
H	3.39525600	1.50724100	1.70962200
H	8.83618000	-4.37017200	-0.03322700
H	7.77185700	-5.26759600	1.07150600
H	7.98911700	-7.29764700	-0.37385000

H	9.03317200	-6.40899500	-1.47912300
H	10.70782500	-6.06742400	0.37577400
H	9.66564600	-6.94876500	1.48342700
H	9.88559200	-9.00687600	0.05663900
H	10.92153000	-8.12669700	-1.05705100
H	12.58625800	-7.74881700	0.78933000
H	11.55124300	-8.62682300	1.90394400
H	13.37655100	-10.11188000	1.04379500
H	11.80331000	-10.71727600	0.50301500
H	12.84459700	-9.83325100	-0.62164900
H	8.25618300	4.34230800	-0.41021400
H	7.04043600	5.11506500	-1.45194700
H	7.00980900	7.10237300	0.06836800
H	8.21078900	6.33814600	1.10389500
H	9.85786000	6.33336600	-0.80709100
H	8.65845200	7.09060500	-1.84602300
H	8.59688700	9.08855000	-0.32041000
H	9.79312000	8.33215100	0.72086400
H	11.43964900	8.31783700	-1.18046600
H	10.24394600	9.07258700	-2.22238400
H	11.83390600	10.78679900	-1.32324600
H	10.20178600	11.10295000	-0.71459400
H	11.40537100	10.34230100	0.33601000
H	2.09679200	1.55699600	-0.95303900
H	-0.34171800	1.41078600	-0.89419100
H	-0.06271000	-2.57094800	0.71910800
H	2.37316900	-2.43418700	0.63721200
H	-2.44160300	1.43529200	0.12946200
H	-8.54952200	-0.10426600	0.22673600
H	-10.15214800	-1.95910200	0.17476600
H	-5.58733800	0.66399200	2.32139700
H	-6.79330300	1.68241600	1.55940500
H	-4.99634000	3.37387500	0.99712000
H	-3.81030900	2.35068200	1.79897400
H	-5.09523900	2.55257600	3.94933100
H	-6.27679100	3.57566400	3.14603900
H	-4.46769800	5.25689500	2.63786600
H	-3.29441300	4.23549500	3.45543300
H	-4.59384400	4.46148900	5.59841900
H	-5.76392700	5.48400700	4.78028200
H	-4.11343800	6.88000100	6.04455700
H	-3.95357500	7.18765200	4.30826400
H	-2.77643400	6.15803900	5.13600500
H	-4.84610900	2.33500700	-1.05424700
H	-5.47618700	0.98397500	-1.97566500
H	-7.81086300	1.58262000	-1.28298300

H	-7.19697700	2.93385900	-0.33756700
H	-6.23267500	3.95319500	-2.41769500
H	-6.83750200	2.60155900	-3.36376000
H	-9.19310300	3.19612600	-2.71508800
H	-8.59345400	4.54321800	-1.75885700
H	-7.61976100	5.58159100	-3.83131200
H	-8.21552300	4.23440400	-4.78756200
H	-9.76790400	6.19357500	-4.96331400
H	-10.59287700	4.84047000	-4.17453400
H	-9.99401300	6.19585800	-3.20741700
H	-12.99968200	-3.51819300	0.20808200

1 2 1.0 3 1.0 4 1.0
2 29 1.5 33 1.5
3 5 1.5 9 1.5
4 10 1.5 14 1.5
5 6 1.5 64 1.0
6 7 1.5 65 1.0
7 8 1.5 15 1.0
8 9 1.5 66 1.0
9 67 1.0
10 11 1.5 68 1.0
11 12 1.5 69 1.0
12 13 1.5 16 1.0
13 14 1.5 70 1.0
14 71 1.0
15 17 1.0
16 23 1.0
17 18 1.0 72 1.0 73 1.0
18 19 1.0 74 1.0 75 1.0
19 20 1.0 76 1.0 77 1.0
20 21 1.0 78 1.0 79 1.0
21 22 1.0 80 1.0 81 1.0
22 82 1.0 83 1.0 84 1.0
23 24 1.0 85 1.0 86 1.0
24 25 1.0 87 1.0 88 1.0
25 26 1.0 89 1.0 90 1.0
26 27 1.0 91 1.0 92 1.0
27 28 1.0 93 1.0 94 1.0
28 95 1.0 96 1.0 97 1.0
29 30 2.0 98 1.0
30 31 1.5 99 1.0
31 32 1.5 34 1.0
32 33 1.5 100 1.0
33 101 1.0
34 35 1.0 38 1.5

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36 37 1.5 39 1.5
37 38 1.5 41 1.0
38 102 1.0
39 40 1.5 42 1.0
40 41 1.0 44 1.5
41 47 1.0 53 1.0
42 43 1.0
43 44 1.5 45 1.5
44 103 1.0
45 46 2.0 104 1.0
46 59 1.0 62 1.5
47 48 1.0 105 1.0 106 1.0
48 49 1.0 107 1.0 108 1.0
49 50 1.0 109 1.0 110 1.0
50 51 1.0 111 1.0 112 1.0
51 52 1.0 113 1.0 114 1.0
52 115 1.0 116 1.0 117 1.0
53 54 1.0 118 1.0 119 1.0
54 55 1.0 120 1.0 121 1.0
55 56 1.0 122 1.0 123 1.0
56 57 1.0 124 1.0 125 1.0
57 58 1.0 126 1.0 127 1.0
58 128 1.0 129 1.0 130 1.0
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61 131 1.0
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Table SI12. Optimized geometry coordinates WN3.1 corresponding to Figure SI4b.

C	-2.11668200	-0.43257800	-0.06880100
C	-1.66117500	-1.73016400	0.24528800
C	-0.20424800	-1.73932900	0.20433800
C	0.24902300	-0.44548300	-0.13601700
C	-0.93492300	0.51158600	-0.33807100
C	0.71185500	-2.77241400	0.42408100
C	2.07229800	-2.51802900	0.28986700
C	2.54566100	-1.23769700	-0.06581300
C	1.60654800	-0.20428500	-0.28532800
C	-3.47432900	-0.14439300	-0.05392900
C	-4.40747400	-1.15704600	0.25862000
C	-3.93957400	-2.45455400	0.55421000
C	-2.57885900	-2.74010600	0.54639700
C	-0.89084300	1.04112800	-1.80515600
C	-1.99777800	2.00404800	-2.25629600
C	-1.77714700	2.50386200	-3.69196600
C	-2.87571600	3.45545600	-4.18268000
C	-2.65510000	3.95853300	-5.61515800
C	-3.75600400	4.90812600	-6.09856700
C	-0.98019900	1.65326600	0.72556400
C	0.11850100	2.72471500	0.68762700
C	-0.10627900	3.80846700	1.75234700
C	0.98040700	4.89136000	1.77019400
C	0.75022900	5.96696200	2.83940700
C	1.83978900	7.04399300	2.85927100
N	-5.78889600	-0.86977300	0.28360400
C	-6.25333800	0.41479100	0.69461900
C	-6.74632800	-1.86614200	-0.06818300
C	-7.86968700	-2.09351500	0.73352300
C	-8.82700900	-3.04798800	0.38291600
C	-8.65847600	-3.81251500	-0.77748700
C	-7.52926300	-3.59582400	-1.58218100
C	-6.59414000	-2.62974600	-1.23912600
C	-7.22022100	1.09748300	-0.05050100
C	-7.70327300	2.34224900	0.35966600
C	-7.20129800	2.93684500	1.52327300
C	-6.22325900	2.26216300	2.27030700
C	-5.76548200	1.01547000	1.86860200

O	-7.59198700	4.14937800	2.01355300
O	-9.52232900	-4.77764600	-1.21019900
C	-10.69298500	-5.04220000	-0.44022800
C	-11.47892900	-6.14083200	-1.14294600
C	-12.77337900	-6.49948300	-0.40185400
C	-13.57967700	-7.60609500	-1.09394100
C	-14.87924800	-7.96322700	-0.36133000
C	-15.67936800	-9.06945300	-1.05644300
C	-8.59670600	4.88282100	1.31578000
C	-8.85536200	6.16665100	2.09245800
C	-9.93543900	7.04335600	1.44569300
C	-10.20644000	8.33469800	2.22822400
C	-11.29021800	9.21780600	1.59658100
C	-11.55750200	10.50213700	2.38778000
C	3.98197600	-1.00303300	-0.20057200
C	5.02404000	-1.68533900	0.41115800
C	6.29897700	-1.20526700	0.03953700
C	6.22683700	-0.13639200	-0.84657100
S	4.59737900	0.27152000	-1.26145900
C	7.75255500	-1.50997900	0.41735100
C	8.46860000	-0.44089100	-0.41488700
C	7.54596500	0.33247900	-1.12921500
C	9.78532300	-0.06330100	-0.68688800
C	9.88860700	1.00921100	-1.58598300
S	8.27647700	1.54193400	-2.11368600
C	8.21018500	-2.92089100	-0.05889800
C	7.55174300	-4.12717700	0.62346100
C	8.08073200	-5.46313500	0.08128600
C	7.43353900	-6.68758500	0.74079100
C	7.96307200	-8.02379700	0.20429900
C	7.31058000	-9.24142600	0.86671500
C	7.93222400	-1.28578200	1.94948000
C	9.34173800	-1.49693200	2.51867600
C	9.40101800	-1.23421400	4.03048800
C	10.79771200	-1.43569900	4.63243700
C	10.85669400	-1.16652700	6.14164800
C	12.25347500	-1.36999200	6.73749000
C	11.12409400	1.57009400	-1.99902700
C	11.40939700	2.61027700	-2.85200900
C	12.79925300	3.02265600	-3.13663200
O	13.11773000	3.93175200	-3.87584700
O	13.72484200	2.26955100	-2.47565700
C	10.39994000	3.36438400	-3.51928100
N	9.55285800	3.96257600	-4.05038400
H	0.37123300	-3.77297000	0.67768700
H	2.78272200	-3.32776200	0.42706200

H	1.96353300	0.78453300	-0.55715000
H	-3.83853900	0.85324000	-0.27012800
H	-4.65382900	-3.23088400	0.80615000
H	-2.24099700	-3.74251400	0.79775400
H	0.07916400	1.53400900	-1.95364300
H	-0.88606600	0.16922800	-2.47246100
H	-2.97297800	1.50540500	-2.20108600
H	-2.05119300	2.87017500	-1.58246200
H	-0.80282500	3.01079800	-3.75563600
H	-1.71428500	1.64081300	-4.37110400
H	-3.85020000	2.94803200	-4.12283200
H	-2.94128500	4.31776500	-3.50225600
H	-1.68188400	4.46618600	-5.67452000
H	-2.58959600	3.09718200	-6.29504900
H	-3.56901000	5.25001000	-7.12295600
H	-4.73715600	4.41737800	-6.08500900
H	-3.82247300	5.79631500	-5.45802200
H	-1.95447300	2.15140600	0.63692900
H	-0.97853900	1.18080900	1.71679700
H	1.09987000	2.26362400	0.85381800
H	0.15911300	3.19921800	-0.30236600
H	-1.08648500	4.28054000	1.58868000
H	-0.16103300	3.33407700	2.74343500
H	1.96131200	4.42107800	1.93478400
H	1.03642100	5.37003000	0.78106100
H	-0.22871800	6.43881900	2.67289200
H	0.69131700	5.48739700	3.82695800
H	1.64642000	7.79551100	3.63335600
H	2.82587400	6.60656500	3.05854600
H	1.89976000	7.56590600	1.89621800
H	-8.00201700	-1.51175000	1.64046600
H	-9.68652500	-3.19301900	1.02714300
H	-7.41453100	-4.18840400	-2.48456100
H	-5.73205200	-2.46149600	-1.87716500
H	-7.60675700	0.64679300	-0.95949300
H	-8.45608100	2.83936400	-0.24140100
H	-5.84915400	2.72962900	3.17591900
H	-5.02018700	0.49636000	2.46329700
H	-10.41061600	-5.35572300	0.57604300
H	-11.29785000	-4.12711000	-0.35224800
H	-11.70755000	-5.80968600	-2.16413100
H	-10.83825600	-7.02720300	-1.23569000
H	-12.53405900	-6.81504500	0.62447800
H	-13.40113100	-5.60120800	-0.30569500
H	-13.81624100	-7.29410400	-2.12188700
H	-12.95556300	-8.50717100	-1.18625500

H	-14.64223100	-8.27328600	0.66641700
H	-15.50245900	-7.06216700	-0.27055600
H	-16.60197000	-9.29883700	-0.51125700
H	-15.95896600	-8.77579300	-2.07571400
H	-15.09601800	-9.99570200	-1.12816600
H	-8.25701000	5.10626000	0.29332700
H	-9.51492400	4.28120200	1.24017100
H	-9.14914400	5.90126500	3.11621200
H	-7.91341500	6.72466400	2.17101700
H	-9.63710000	7.29801100	0.41800400
H	-10.87030600	6.47002300	1.35868400
H	-10.50035500	8.07990000	3.25715200
H	-9.27307100	8.91055500	2.31327900
H	-10.99499300	9.47480100	0.56929800
H	-12.22184300	8.64062900	1.50949600
H	-12.33573500	11.10987900	1.91246100
H	-11.88799000	10.27686800	3.40922500
H	-10.65281200	11.11807800	2.46191200
H	4.84605500	-2.47722400	1.12917000
H	10.67136300	-0.52968200	-0.26889600
H	8.03358900	-2.98106500	-1.14046500
H	9.29813900	-2.98765000	0.07304200
H	7.72141100	-4.09150300	1.70827000
H	6.46447400	-4.08905900	0.47669000
H	7.91501700	-5.50491800	-1.00516000
H	9.17073000	-5.50731000	0.22402700
H	7.59581900	-6.64436100	1.82833500
H	6.34367300	-6.64566300	0.59516400
H	7.80119700	-8.06683300	-0.88208000
H	9.05175100	-8.06632400	0.35084400
H	7.70987000	-10.17876600	0.46303600
H	7.48456200	-9.24436100	1.94989700
H	6.22527800	-9.24559400	0.70675300
H	7.60423400	-0.26316800	2.17561200
H	7.23315200	-1.94918000	2.47544800
H	9.68374500	-2.52177300	2.32007500
H	10.05076000	-0.82807400	2.01314100
H	9.06255800	-0.20754900	4.23247600
H	8.68623800	-1.89552000	4.54238900
H	11.13561800	-2.46394500	4.43433900
H	11.51395000	-0.77682200	4.11913100
H	10.52023200	-0.13876800	6.33846200
H	10.14023400	-1.82389000	6.65457200
H	12.26234400	-1.16789900	7.81456300
H	12.60193100	-2.39952100	6.58900300
H	12.98612600	-0.70243400	6.26742400

H 11.99175400 1.08541500 -1.55891600
H 14.58706000 2.63607400 -2.74347900

1 2 1.5 5 1.0 10 1.5
2 3 1.0 13 1.5
3 4 1.5 6 1.5
4 5 1.0 9 1.5
5 14 1.0 20 1.0
6 7 1.5 83 1.0
7 8 1.5 84 1.0
8 9 1.5 53 1.0
9 85 1.0
10 11 1.5 86 1.0
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14 15 1.0 89 1.0 90 1.0
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18 19 1.0 97 1.0 98 1.0
19 99 1.0 100 1.0 101 1.0
20 21 1.0 102 1.0 103 1.0
21 22 1.0 104 1.0 105 1.0
22 23 1.0 106 1.0 107 1.0
23 24 1.0 108 1.0 109 1.0
24 25 1.0 110 1.0 111 1.0
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41 42 1.0 123 1.0 124 1.0
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Table SI13. Optimized geometry coordinates WN1 corresponding to Figure SI4c.

C	2.43643800	-0.62350600	-0.36209800
C	1.95735600	-1.87326100	-0.80709800
C	0.50068600	-1.83306400	-0.84311400
C	0.07123100	-0.55372200	-0.42417800
C	1.27271400	0.33837600	-0.07738300
C	-0.43447000	-2.81336300	-1.18605700
C	-1.79162100	-2.51942400	-1.10357200
C	-2.24160400	-1.25880900	-0.66297700
C	-1.28311400	-0.27951700	-0.31288700
C	3.80158100	-0.38834500	-0.27109400
C	4.71683000	-1.41032400	-0.60459900
C	4.22433300	-2.65924900	-1.03774300
C	2.85708500	-2.89040300	-1.13697500
C	1.40965900	1.56315800	-1.03452600
C	0.34082800	2.66222600	-0.95514900
C	0.65739400	3.83976100	-1.88892800
C	-0.39162700	4.95840300	-1.84580200
C	-0.06424700	6.13852100	-2.76973400
C	-1.11245900	7.25489500	-2.72041300
C	1.16672100	0.74462000	1.42562000
C	2.27178900	1.63622800	2.00912000
C	1.98948900	2.02622900	3.46778800
C	3.08441400	2.90367100	4.08768100
C	2.80245200	3.29897900	5.54299000
C	3.90031400	4.17467200	6.15543400
C	-3.66686200	-0.95056400	-0.55912700
N	6.10686100	-1.18638900	-0.50898300
C	6.65283700	0.11175400	-0.73207300
C	6.98951700	-2.24933200	-0.15513400
C	8.16049000	-2.47757900	-0.88491400
C	9.04504400	-3.49886300	-0.53059100
C	8.75305400	-4.32688200	0.55907600
C	7.57644000	-4.10882100	1.29178100
C	6.71374200	-3.07854600	0.94643600
C	7.57169700	0.66477300	0.16565100
C	8.13174100	1.92464200	-0.05761400
C	7.75701700	2.66445300	-1.18472100
C	6.82972600	2.11992700	-2.08623400
C	6.29488800	0.85815600	-1.86891500
O	8.22996800	3.90769200	-1.49620300
O	9.53727300	-5.35992400	0.98849800
C	10.73314100	-5.63284500	0.27726100
C	9.16162100	4.50956500	-0.61264400
C	-4.28679900	0.28546800	-0.58824500
C	-5.69138800	0.22728100	-0.45758100
C	-6.18580200	-1.05810800	-0.32449500

S	-4.86327600	-2.21497000	-0.34725700
C	-7.55016100	-1.49090000	-0.17884500
C	-8.04519300	-2.79153900	-0.16390600
C	-9.43580700	-2.85037800	-0.00275500
C	-10.05154700	-1.60550200	0.11036400
S	-8.84252000	-0.32747200	0.01837900
C	-11.45374200	-1.43037200	0.27813000
C	-12.20921500	-0.29203400	0.40068600
C	-11.64749300	1.01924800	0.37493700
N	-11.16207100	2.07774100	0.35049200
C	-13.67894900	-0.34655800	0.57044700
O	-14.39891300	0.62364100	0.68288200
O	-14.16426100	-1.61912400	0.58972500
H	-0.11321000	-3.79751600	-1.51682300
H	-2.51695800	-3.27342600	-1.39741600
H	-1.62444000	0.67455000	0.07529800
H	4.18500200	0.57318100	0.04917100
H	4.92636300	-3.44052400	-1.30815200
H	2.50158900	-3.85524900	-1.49014100
H	2.39186100	2.01911500	-0.85355700
H	1.44598600	1.17871000	-2.06236600
H	-0.64028600	2.25004600	-1.22266200
H	0.25230500	3.03793800	0.07345300
H	1.64143100	4.25546300	-1.62597400
H	0.75102100	3.46953100	-2.92051900
H	-1.37516600	4.54712400	-2.11829500
H	-0.49174800	5.32476600	-0.81298700
H	0.91940800	6.54743400	-2.49818100
H	0.03359100	5.77321200	-3.80193600
H	-0.84942800	8.08119600	-3.39066000
H	-2.10064500	6.88488000	-3.02034400
H	-1.20753200	7.66526900	-1.70744900
H	1.10714700	-0.17928900	2.01573900
H	0.20246000	1.25013200	1.56836200
H	2.38111600	2.55161400	1.41152400
H	3.23646900	1.11673300	1.96223100
H	1.87003800	1.11406100	4.07091500
H	1.02594500	2.55442400	3.52358900
H	3.20724700	3.81459800	3.48261400
H	4.04753500	2.37416900	4.03619000
H	2.67993500	2.38922300	6.14781600
H	1.84055100	3.82874300	5.59409700
H	3.66911000	4.43941300	7.19355200
H	4.02253800	5.10870600	5.59303500
H	4.86810800	3.65795300	6.15127800
H	8.38708400	-1.84496400	-1.73768200

H	9.94455300	-3.64362500	-1.11816600
H	7.36711600	-4.75268500	2.14038700
H	5.81286800	-2.91039800	1.52845500
H	7.85911500	0.10094800	1.04783900
H	8.84389900	2.31837600	0.65865900
H	6.55529100	2.70005700	-2.96185600
H	5.58923700	0.44055100	-2.58054600
H	11.19454600	-6.48388100	0.78163100
H	11.42371200	-4.77909600	0.30306900
H	10.52988300	-5.89871200	-0.76880200
H	9.39982800	5.48290100	-1.04551900
H	10.08186700	3.91583800	-0.52849000
H	8.73450000	4.65342600	0.38894100
H	-3.74199000	1.21092800	-0.73577500
H	-6.32987300	1.10448700	-0.48095100
H	-7.41305100	-3.66536700	-0.27608100
H	-10.00252900	-3.77544100	0.02891900
H	-12.01040000	-2.36307800	0.31445300
H	-15.12735200	-1.52425600	0.70470400

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2 3 1.0 13 1.5
3 4 1.5 6 1.5
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5 14 1.0 20 1.0
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7 8 1.5 61 1.0
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9 62 1.0
10 11 1.5 63 1.0
11 12 1.5 27 1.0
12 13 1.5 64 1.0
13 65 1.0
14 15 1.0 66 1.0 67 1.0
15 16 1.0 68 1.0 69 1.0
16 17 1.0 70 1.0 71 1.0
17 18 1.0 72 1.0 73 1.0
18 19 1.0 74 1.0 75 1.0
19 76 1.0 77 1.0 78 1.0
20 21 1.0 79 1.0 80 1.0
21 22 1.0 81 1.0 82 1.0
22 23 1.0 83 1.0 84 1.0
23 24 1.0 85 1.0 86 1.0
24 25 1.0 87 1.0 88 1.0
25 89 1.0 90 1.0 91 1.0
26 44 2.0 47 1.0

27 28 1.0 29 1.0
28 35 1.5 39 1.5
29 30 1.5 34 1.5
30 31 1.5 92 1.0
31 32 1.5 93 1.0
32 33 1.5 41 1.0
33 34 1.5 94 1.0
34 95 1.0
35 36 1.5 96 1.0
36 37 1.5 97 1.0
37 38 1.5 40 1.0
38 39 1.5 98 1.0
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40 43 1.0
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42 100 1.0 101 1.0 102 1.0
43 103 1.0 104 1.0 105 1.0
44 45 1.5 106 1.0
45 46 2.0 107 1.0
46 47 1.0 48 1.5
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48 49 1.5 52 1.0
49 50 1.5 108 1.0
50 51 1.5 109 1.0
51 52 1.0 53 1.5
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53 54 2.0 110 1.0
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Table SI14. Optimized geometry coordinates WN3 corresponding to Figure SI4d.

C	-3.89620300	0.44975200	-0.28535300
C	-3.38958200	1.69213700	-0.72027600
C	-1.93467900	1.61693000	-0.76458900
C	-1.53398900	0.32309300	-0.36386800

C	-2.75429400	-0.54198400	-0.01464600
C	-0.97797800	2.57739300	-1.10654900
C	0.37161700	2.24933100	-1.04076900
C	0.79446100	0.97328000	-0.61352300
C	-0.18518700	0.01403900	-0.26935100
C	-5.26623300	0.24585600	-0.19199400
C	-6.15852400	1.29149500	-0.51443300
C	-5.63829200	2.53269500	-0.93721700
C	-4.26621700	2.73303700	-1.03768700
C	-2.92852600	-1.75934700	-0.97521600
C	-1.89070300	-2.88840000	-0.90328100
C	-2.24142600	-4.05278800	-1.84154300
C	-1.22517800	-5.20123400	-1.79953700
C	-1.58115800	-6.36677600	-2.73144700
C	-0.56594600	-7.51318400	-2.68083400
C	-2.64708200	-0.95654600	1.48619500
C	-3.77452700	-1.81391100	2.07788200
C	-3.49461200	-2.20866800	3.53571000
C	-4.61211300	-3.04920800	4.16629700
C	-4.33437900	-3.44376800	5.62261100
C	-5.45531700	-4.28082100	6.24710200
C	2.22147400	0.67051700	-0.52500400
N	-7.55316100	1.09796600	-0.41905200
C	-8.12854800	-0.18605400	-0.65067400
C	-8.41324900	2.17943900	-0.06639400
C	-9.57569800	2.43539700	-0.80062600
C	-10.43855600	3.47567000	-0.44818000
C	-10.13281600	4.29499100	0.64421700
C	-8.96462400	4.04912800	1.38159300
C	-8.12380300	3.00029400	1.03797500
C	-9.05931400	-0.72356400	0.24413400
C	-9.64825700	-1.96875000	0.01323200
C	-9.29136300	-2.70959800	-1.11899700
C	-8.35232500	-2.18075200	-2.01768100
C	-7.78845600	-0.93304300	-1.79258800
O	-9.79309200	-3.93950000	-1.43802000
O	-10.89581200	5.34464700	1.07198100
C	-12.08271600	5.64405400	0.35645700
C	-10.73667300	-4.52591600	-0.55676400
C	3.27613700	1.55266500	-0.33730000
C	4.53746800	0.91809900	-0.32009200
C	4.44101600	-0.46008600	-0.47639800
S	2.80688200	-0.99108400	-0.67968800
C	5.99283800	1.34718000	-0.10452800
C	6.68170500	-0.01989800	-0.17623600
C	5.74457400	-1.03730400	-0.39127700

C	7.98654800	-0.51582500	-0.13145000
C	8.06487000	-1.90833900	-0.28651800
S	6.44503000	-2.60569400	-0.51237600
C	9.28391600	-2.63296400	-0.26161500
C	9.54408900	-3.97707300	-0.39005200
C	6.52499500	2.24961600	-1.25825300
C	5.90882900	3.64994400	-1.37567800
C	6.49825400	4.45245400	-2.54489900
C	5.89587900	5.85646600	-2.68329800
C	6.47874400	6.66182800	-3.85179000
C	5.87217900	8.06277400	-3.98139800
C	6.12364100	2.00367900	1.30297700
C	7.52664800	2.46166600	1.72290300
C	7.54162900	3.07601200	3.13032300
C	8.93354000	3.53846000	3.57975200
C	8.95109200	4.14944600	4.98685400
C	10.34476000	4.60644500	5.42959900
C	10.92047400	-4.51093200	-0.33180500
O	11.21688200	-5.68364800	-0.43746800
O	11.86091100	-3.54110800	-0.14269700
C	8.51962300	-4.94914800	-0.58604900
N	7.66032200	-5.71966700	-0.74527400
H	-1.27815100	3.57126600	-1.42838400
H	1.11462200	2.98266100	-1.33972500
H	0.13306900	-0.95588300	0.10138500
H	-5.67079900	-0.70953800	0.12051800
H	-6.32248100	3.33235000	-1.19940100
H	-3.88937300	3.69255100	-1.38329500
H	-3.92231600	-2.18834200	-0.79145600
H	-2.95862100	-1.37025900	-2.00155500
H	-0.89826400	-2.50458500	-1.17046500
H	-1.81145700	-3.27129100	0.12338200
H	-3.23785500	-4.44027300	-1.58168300
H	-2.32211400	-3.67626500	-2.87198700
H	-0.22907000	-4.81671600	-2.06425300
H	-1.14093900	-5.57578700	-0.76830600
H	-2.57818300	-6.74837100	-2.46836400
H	-1.66151600	-5.99364200	-3.76242400
H	-0.84811000	-8.32809300	-3.35728800
H	0.43461300	-7.17047000	-2.97144300
H	-0.48989200	-7.93121800	-1.66944800
H	-1.69797600	-1.49268600	1.61796300
H	-2.55323900	-0.03677100	2.07848500
H	-4.72343800	-1.26574900	2.03591200
H	-3.91485500	-2.72679000	1.48299000
H	-2.54759800	-2.76632300	3.58672600

H	-3.34280200	-1.29865900	4.13497900
H	-5.55920300	-2.49132600	4.11654100
H	-4.76543000	-3.95967600	3.56758200
H	-3.38902600	-4.00261900	5.67202700
H	-4.18042400	-2.53419000	6.22059400
H	-5.22656600	-4.54558100	7.28577900
H	-6.40666700	-3.73436200	6.24461400
H	-5.60970000	-5.21443800	5.69197900
H	-9.81295400	1.80967100	-1.65557700
H	-11.33201600	3.64137300	-1.03944600
H	-8.74458800	4.68652200	2.23238700
H	-7.22932300	2.81102400	1.62339400
H	-9.33287400	-0.15897800	1.13024900
H	-10.36871200	-2.35073900	0.72757300
H	-8.09157200	-2.76151600	-2.89704400
H	-7.07348500	-0.52740200	-2.50182800
H	-12.52785000	6.50409700	0.86019500
H	-12.79144600	4.80521300	0.37829900
H	-11.86977200	5.90689400	-0.68845900
H	-10.99726400	-5.49091000	-0.99536400
H	-10.31135900	-4.68563500	0.44317800
H	-11.64322500	-3.91219700	-0.46741700
H	3.11422500	2.61271800	-0.18129400
H	8.88169300	0.08228200	0.00330700
H	10.16049800	-2.00712800	-0.11530600
H	7.61207200	2.34806100	-1.13931900
H	6.37246800	1.70965500	-2.20147200
H	4.82288400	3.56711500	-1.51348100
H	6.06283200	4.21176900	-0.44430600
H	7.58780100	4.53561100	-2.41719000
H	6.34390000	3.89606200	-3.48089200
H	4.80594200	5.77354800	-2.80940200
H	6.05101300	6.41341700	-1.74705300
H	7.56780400	6.74448400	-3.72670300
H	6.32199700	6.10658100	-4.78740500
H	6.30898500	8.61143200	-4.82350200
H	4.78834800	8.01228100	-4.14322200
H	6.04324800	8.65454900	-3.07364800
H	5.44174200	2.86324200	1.34264400
H	5.74520000	1.28531300	2.04133700
H	8.21813300	1.60900300	1.70020700
H	7.91710500	3.19879500	1.00800900
H	6.84757500	3.92904600	3.16207600
H	7.15263900	2.34136400	3.85035500
H	9.62810000	2.68567200	3.54729100
H	9.32327400	4.27441700	2.86047800

H	8.25839500	5.00249600	5.01984400
H	8.56142100	3.41415200	5.70502200
H	10.32304800	5.03795500	6.43674300
H	11.05181500	3.76779400	5.44201700
H	10.74724400	5.36763400	4.74980500
H	12.71226500	-4.01472600	-0.12302400

1 2 1.5 5 1.0 10 1.5
2 3 1.0 13 1.5
3 4 1.5 6 1.5
4 5 1.0 9 1.5
5 14 1.0 20 1.0
6 7 1.5 73 1.0
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8 9 1.5 26 1.0
9 75 1.0
10 11 1.5 76 1.0
11 12 1.5 27 1.0
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13 78 1.0
14 15 1.0 79 1.0 80 1.0
15 16 1.0 81 1.0 82 1.0
16 17 1.0 83 1.0 84 1.0
17 18 1.0 85 1.0 86 1.0
18 19 1.0 87 1.0 88 1.0
19 89 1.0 90 1.0 91 1.0
20 21 1.0 92 1.0 93 1.0
21 22 1.0 94 1.0 95 1.0
22 23 1.0 96 1.0 97 1.0
23 24 1.0 98 1.0 99 1.0
24 25 1.0 100 1.0 101 1.0
25 102 1.0 103 1.0 104 1.0
26 44 1.5 47 1.0
27 28 1.0 29 1.0
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30 31 1.5 105 1.0
31 32 1.5 106 1.0
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33 34 1.5 107 1.0
34 108 1.0
35 36 1.5 109 1.0
36 37 1.5 110 1.0
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38 39 1.5 111 1.0
39 112 1.0

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42 113 1.0 114 1.0 115 1.0
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48 49 1.0 56 1.0 62 1.0
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54 55 2.0 121 1.0
55 68 1.0 71 1.5
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57 58 1.0 124 1.0 125 1.0
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63 64 1.0 137 1.0 138 1.0
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65 66 1.0 141 1.0 142 1.0
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67 145 1.0 146 1.0 147 1.0
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Table SI15. Optimized geometry coordinates D21L6 corresponding to Figure SI4e.

C	-1.39410100	0.64481200	0.56844100
C	-2.02393800	-0.54607000	0.15771000
C	-0.01400700	0.77834200	0.56649600
C	0.81452600	-0.28146300	0.14426600
C	0.19224500	-1.47819800	-0.26844000
C	-1.18846300	-1.60167200	-0.25963000
N	2.21115800	-0.14592600	0.13153100
C	2.81914600	1.13370000	-0.05418000
C	3.06275300	-1.28495600	0.26513800
C	2.88204200	-2.20331100	1.31376200
C	3.72243800	-3.29978900	1.44690800
C	4.78295200	-3.49795600	0.54878700
C	4.97811100	-2.58108800	-0.49146900
C	4.11493600	-1.49289100	-0.63152000
C	2.43374100	1.96774200	-1.11782900
C	3.04045500	3.20152700	-1.30528700
C	4.06704000	3.62800600	-0.44807500
C	4.46499300	2.79921000	0.60804700
C	3.83469400	1.56839700	0.80236900
O	4.60687600	4.84850900	-0.72889700
O	5.55820900	-4.59755500	0.77437300
C	-3.47458300	-0.69792500	0.15539300
C	-4.22314900	-1.86159900	0.18693600
C	-5.61806000	-1.64817600	0.16880000
C	-5.97861700	-0.31281900	0.12330200
S	-4.53832300	0.69496600	0.08398600

C	5.67840500	5.33055700	0.08093900
C	6.10905000	6.68109800	-0.47484800
C	7.27734600	7.29524100	0.30692700
C	7.72110200	8.65538800	-0.24708700
C	8.89652800	9.27402300	0.52019100
C	9.33419900	10.63119900	-0.03992700
C	6.66547700	-4.84215800	-0.09184300
C	7.36686600	-6.10789500	0.38197600
C	8.59062800	-6.44817700	-0.47800000
C	9.31241200	-7.72539300	-0.02839100
C	10.54288400	-8.06003000	-0.88080000
C	11.25913900	-9.33772000	-0.43151000
C	-7.29334100	0.26858100	0.10407700
C	-7.64292400	1.61365300	0.18815100
C	-9.02628500	1.82800300	0.13973400
C	-9.78230500	0.66346500	0.01748200
S	-8.71696000	-0.73887000	-0.04601200
C	-11.20298900	0.64759600	-0.04772400
C	-12.08712100	-0.39534400	-0.16515100
C	-11.67404300	-1.75847500	-0.24611800
N	-11.30950900	-2.86291700	-0.31012100
C	-13.54949000	-0.17413900	-0.21672300
O	-14.38011100	-1.05292500	-0.31932600
O	-13.89061800	1.14253700	-0.13669600
H	-1.99604200	1.47485600	0.92951200
H	0.43503800	1.70443500	0.90792700
H	0.80098900	-2.30491600	-0.61751900
H	-1.63182100	-2.52491400	-0.62108300
H	2.07514700	-2.05096100	2.02417500
H	3.58729900	-4.01210900	2.25487100
H	5.78580100	-2.70737300	-1.20281000
H	4.26735900	-0.79095500	-1.44562500
H	1.65272700	1.64085900	-1.79764000
H	2.74764400	3.84943000	-2.12560300
H	5.25139900	3.10184400	1.28983000
H	4.14328600	0.93293900	1.62688900
H	-3.77470600	-2.84603200	0.25677200
H	-6.34530300	-2.45265900	0.21026800
H	5.34568900	5.42611100	1.12525800
H	6.51413200	4.61530500	0.05872900
H	6.38749800	6.55177200	-1.52863900
H	5.24584700	7.35884300	-0.45894500
H	6.99432700	7.40963600	1.36375000
H	8.13205900	6.60282300	0.29332500
H	7.99766300	8.54276100	-1.30576600
H	6.86900300	9.35073400	-0.22839700

H	8.61972700	9.38625200	1.57817900
H	9.74738600	8.57817000	0.50097700
H	10.17491600	11.04566500	0.52778800
H	9.64945000	10.54483300	-1.08704600
H	8.51472800	11.35937900	-0.00093700
H	6.31178700	-4.95891600	-1.12709700
H	7.35408800	-3.98428600	-0.06769800
H	7.66620000	-5.97305000	1.42926400
H	6.64840000	-6.93736600	0.36374100
H	8.28204100	-6.55871300	-1.52811200
H	9.29858100	-5.60648900	-0.45574400
H	9.61676900	-7.62023800	1.02340100
H	8.60880100	-8.57030900	-0.05800700
H	10.23822000	-8.16121100	-1.93219200
H	11.24566400	-7.21530800	-0.84824200
H	12.13435600	-9.54659400	-1.05705700
H	11.60381000	-9.25500600	0.60662800
H	10.59303400	-10.20730900	-0.48980400
H	-6.91180200	2.40765900	0.29181200
H	-9.48856500	2.80834100	0.19629900
H	-11.65464300	1.63478100	0.00453100
H	-14.86402700	1.15732900	-0.18074100

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5. References

- (1) Li, R.; Liu, J.; Cai, N.; Zhang, M.; Wang, P. *The journal of physical chemistry. B* **2010**, *114*, 4461–4.
- (2) Tsao, H. N.; Yi, C.; Moehl, T.; Yum, J.-H.; Zakeeruddin, S. M.; Nazeeruddin, M. K.; Grätzel, M. *ChemSusChem* **2011**, *4*, 591–4.