Supplementary Information for:

True absolute determination of photoluminescence quantum yields by coupling multiwavelength thermal lens and photoluminescence spectroscopies

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SI1 Details on the synthesis of the novel materials

3-(4-(dimethylamino)phenyl)-6-phenyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione

Under reflux temperature, nitrogen atmosphere and vigorous stirring 2,3-dihydro-2-oxo-5phenyl-1H-pyrrole-4-carboxylic acid ethyl ester (0.90 g, 3.92 mmol) was added to a solution of sodium t-amyloxide (obtained from 0.28 g, 12.02 mmol sodium metal dissolved in 40 ml of dry t-amyl alcohol). 4-dimethylbenzonitrile (0.40 g, 2.70 mmol) was added dropwise over 1 hour. The mixture was stirred under reflux for 15 hours and after cooling, cold methanol and hydrochloric acid were added. The dark violet precipitate was filtered, washed with methanol and water and dried under vacuum to give a purple solid that was used in the next step without further purification (0.18 g, 28 %).

2,5-dibenzyl-3,6-bis(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)-2,5-dihydropyrrolo[3,4c]pyrrole-1,4-dione (TPADPP)

A stirred mixture of 2,5-dibenzyl-3,6-bis(4-bromophenyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-K₂CO₃ 1,4-dione (0.35)0.55 mmol), (1.40)10.13 mmol), g, g, Pd(PPh₃)₄ (0.013g, 0.011 mmol), THF (7 mL) and water (3 mL) was heated at reflux for 30 mins under nitrogen. After cooling to 40 °C, а solution of 4-(diphenylamino)phenyl boronic acid (0.48 g, 1.65 mmol) in THF (5 mL) was added via syringe. The resulting mixture was heated under reflux for 24 hours, after which time, water (30 mL) was added and the product extracted with dichloromethane. The dichloromethane solution was dried over anhydrous MgSO₄, evaporated and the crude product purified by wet flash chromatography on silica, eluting with dichloromethane/hexane to give a dark red solid (0.28 g, 53%). ¹H NMR (CDCl₃): $\delta = 5.05$ (s, 4H, CH₂), 7.03-7.06 (t, 4H, ArH), 7.10-7.14 (m, 12H, ArH), 7.24-7.34 (m, 18H, ArH), 7.46-7.48 (d, 4H, ArH), 7.61-7.63 (d, 4H, ArH), 7.84-7.86 (d, 4H, ArH), ¹³C NMR (CDCl₃): δ = 45.9 (CH₂), 109.7 (C=C), 123.3 (C=C), 123.4 (C=C), 124.8 (C=C), 126.1 (C=C), 126.7 (C=C), 126.8 (C=C), 127.4 (C=C), 127.8 (C=C), 128.9 (C=C), 129.4 (C=C), 129.7 (C=C), 133.2 (C=C), 137.7 (C=C), 143.5 (C=C), 147.4 (C=C), 148.1 (C=C), 148.6 (C=C), 163.0 (C=O), IR (ATR)/ cm⁻¹: 3033 (ArH), 1666 (C=O), 1585 (ArH), 1495 (ArH), 1451 (ArH), 1326 (CN) 822 (ArH), 746 (ArH), 726 (ArH), Anal. Calcd for C₆₈H₅₀N₄O₂: C, 85.51; H, 5.28; N, 5.87. Found: C, 85.26; H, 5.16; N, 5.65.



Figure S1.1 ¹H-NMR (400 MHz) spectrum for TPADPP in CDCl₃.



Scheme S1.1 TPADPP synthetic route. (a) K_2CO_3 , $Pd(Ph_3)_4$, THF/water, 4-(diphenylamino)phenyl boronic acid

2,5-dibenzyl-3-(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)-6-phenyl-2,5-dihydropyrrolo-[3,4-c]pyrrole-1,4-dione (mTPADPP)

A stirred mixture of 2,5-dibenzyl-3-(4-bromophenyl)-6-phenyl-2,5-dihydropyrrolo[3,4c]pyrrole-1,4-dione (0.20)0.36 mmol), K₂CO₃ (0.10)g, 0.36 mmol), g, Pd(PPh₃)₄ (0.0047g, 0.0004 mmol), THF (7 mL) and water (3 mL) was heated at reflux for 30 solution mins under nitrogen. After cooling to 40 °C, а of 4-(diphenylamino)phenyl boronic acid (0.104 g, 0.36 mmol) in THF (5 mL) was added via syringe. The resulting mixture was heated under reflux for 24 hours, after which time, water (30 mL) was added and the product extracted with dichloromethane. The dichloromethane solution was dried over anhydrous MgSO₄, evaporated and the crude product purified by wet flash chromatography on silica, eluting with dichloromethane/hexane to give an orange solid (0.18 g, 69%). ¹H NMR (CDCl₃): δ = 4.99 (s, 2H, CH₂), 5.03 (s, 2H, CH₂), 7.02-7.33 (m, 23H, ArH), 7.40-7.49 (m, 4H, ArH), 7.61-7.63 (d, 2H, ArH), 7.74-7.75 (d, 2H, ArH), 7.83-7.85 (d, 2H, ArH), ¹³C NMR (CDCl₃): $\delta = 45.7$ (CH₂), 45.8 (CH₂), 109.6 (C=C), 109.8 (C=C), 123.3 (C=C), 123.4 (C=C), 124.8 (C=C), 126.7 (C=C), 126.8 (C=C), 127.4 (C=C), 127.8 (C=C), 128.0 (C=C), 128.8 (C=C), 128.9 (C=C), 128.9 (C=C), 129.1 (C=C), 129.4 (C=C), 129.7 (C=C), 131.4 (C=C), 137.6 (C=C), 137.6 (C=C), 143.6 (C=C), 147.4 (C=C), 148.1 (C=C), 148.6 (C=C), 149.0 (C=C), 150.8 (C=C), 154.7 (C=C), 154.8 (C=C), 157.1 (C=C), 162.9 (C=O), 163.0 (C=O), IR (ATR)/ cm⁻¹: 3033 (ArH), 2943 (CH), 1677 (C=O), 1590 (ArH), 1491 (ArH), 1326 (CN), 1270 (CN), 821 (ArH), 736 (ArH), 690 (ArH), Anal. *Calcd for* C₅₀H₃₇N₃O₂: C, 84.36; H, 5.24; N, 5.90. *Found*: C, 83.60; H, 5.21; N, 5.78.



Figure S1.2 ¹H-NMR (400 MHz) spectrum for mTPADPP in CDCl₃.



Scheme S1.2 (a) mTPADPP synthetic route. (a) K_2CO_3 , $Pd(Ph_3)_4$, THF/water, 4-(diphenylamino)phenyl boronic acid

2,5-dibenzyl-3-(4-(dimethylamino)phenyl)-6-phenyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (mDMADPP)

A suspension of 3-(4-(dimethylamino)phenyl)-6-phenyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (0.20 g, 0.60 mmol) and K₂CO₃ (1.00 g, 0.60 mmol) in dry DMF (20 mL) was heated at 120 °C under nitrogen. Under vigorous stirring, benzyl bromide (2.4 mL, 20.00 mmol) in DMF (10 mL) was added dropwise over 30 mins. Stirring and heating at 120 °C were continued for 1 hour. After cooling to room temperature, cold methanol and water was added to give an orange precipitate that was collected by filtration and washed with water and dried (0.14 g, 45 %).¹H NMR (CDCl₃): δ = 3.03 (s, 6H, CH₃), 5.01 (s, 2H, CH₂), 5.04 (s, 2H, CH₂), 6.65-6.67 (d, 2H, ArH), 7.19-7.41 (m, 13H, ArH), 7.70-7.72 (d, 2H, ArH) 7.84-7.86 (d, 2H, ArH), ¹³C NMR (CDCl₃): δ = 29.79 (CH₃), 40.1 (CH₃), 45.7 (CH₂), 46.1 (CH₂), 107.1 (C=C), 111.5 (C=C), 114.9 (C=C), 126.8 (C=C), 127.2 (C=C), 128.7 (C=C), 128.8 (C=C), 128.8 (C=C), 129.0 (C=C), 137.9 (C=C), 138.0 (C=C), 145.5 (C=C), 150.9 (C=C), 152.4 (C=C), 162.7 (C=O), 163.6 (C=O), IR (ATR)/ cm⁻¹: 3031 (ArH), 2943 (CH), 1666 (C=O), 1602 (NH), 1569 (NH), 1592 (C=C), 1516 (C=C), 1487 (C=C), 1205 (CN), 1174 (CN) 824 (ArH), 736 (ArH) 691 (ArH), *Anal. Calcd for* C₃₄H₂₉N₃O₂: C, 79.82; H, 5.57; N, 8.21. *Found:* C, 79.73; H, 5.93; N, 7.65.



Figure S1.3 ¹H-NMR (400 MHz) spectrum for mDMADPP in CDCl₃.



Scheme S1.3 mDMADPP synthetic route. (a) Na, t-amyl alcohol, 4-dimethylaminobenzonitrile. (b) BnBr, K₂CO₃, DMF, 120 °C