Supporting Information

Methyl-shield strategy enables efficient blue thermally activated

delayed fluorescent hosts for high-performance fluorescent OLEDs

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I. General remarks

NMR spectra were obtained on an Agilent 400-MR DD2. The ¹H NMR (400 MHz) chemical shifts were measured relative to CDCl₃ as the internal reference (CDCl₃: δ = 7.26 ppm). The ¹³C NMR (100 MHz) chemical shifts were given using CDCl₃ as the internal standard (CDCl₃: $\delta = 77.16$ ppm,). High resolution mass spectra (HR-MS) were obtained with a Shimadzu LCMS-IT-TOF (ESI). X-Ray single-crystal diffraction data were collected on an Agilent Technologies Gemini plus single crystal diffraction. Thermogravimetric analysis (TGA) was carried out using DTG-60(H) at a rate of 10 °C/min under nitrogen atmosphere. Cyclic voltammograms were performed on LK2005A with a solution of tetrabutylammonium hexafluorophosphate (Bu₄NPF₆, 0.1 M) in DCM as electrolyte and ferrocene/ferrocenium (Fc/Fc^+) as standard. UV-visible absorption spectra were obtained on a HITACHI U-2910 spectrometer. Fluorescence spectra, phosphorescence spectra and photoluminescence quantum yield were collected on a Horiba Jobin Yvon-Edison Fluoromax-3 fluorescence spectrometer with a calibrated integrating sphere system. Transient PL decay spectra were obtained with Horiba Single Photon Counting Controller: FluoroHub and Horiba **TBX** Picosecond Photon Detection.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. The solvents were dried with an innovative technology solvent purification system (model no.:PS-MD-5).

Device fabrication and performance measurement: ITO substrates were cleaned in the ultrasonic bath using alkaline detergent and deionized water, and then treated with O2 plasma for 10 min before device fabrication. Organic layers, LiF and Al were deposited on ITO substrates by thermal evaporation in a vacuum chamber under the vacuum of pressure around 6×10^{-6} mbar. Current density versus voltage (J-V) and luminance versus voltage (L-V) characteristics of OLEDs was measured by Keithley B1500A and model DLM-100Z photometer, respectively. The EL spectra and CIE 1931 coordinates were obtained using an OPT2000 spectrophotometer.

II. Synthesis and characterization

(i) Synthesis of ACRXTO



3-Bromo-9*H***-xanthen-9-one.** Pyridine (0.4 mL, 5 mmol) and DMF (10 mL) were added to a mixture of 4-bromo-2-iodobenzoic acid (1.6 g, 5 mmol), phenol (940 mg, 10 mmol), copper (47.6 mg, 0.75 mmol), CuI (47.5 mg, 0.25 mmol), and K_2CO_3 (1.0 g, 7.5 mmol) under a N₂ atmosphere. The reaction mixture was stirred at 100 °C for

24 h. The resulting solution was cooled to ambient temperature, diluted with brine solution and ethyl acetate, and acidified by concentrated HCl to pH = 1. The organic extracts were washed with water, dried over Na₂SO₄ and concentrated under reduced pressure. The resulting residue was treated with triflic acid (5 mL) at 100 °C for 3 h. After that, it was allowed to cool to room temperature and quenched with water. The mixture was extracted with dichloromethane (DCM) and organic phase was separated, dried over Na₂SO₄, filtered, and evaporated under vacuum. Purification by column chromatography on silica gel (petroleum ether/dichloromethane = 5/1, v/v) afforded **3-bromo-9H-xanthen-9-one** as a white solid (760 mg, 55 % yield). ¹H NMR (400 MHz, CDCl₃): δ = 7.41 (t, *J* = 8.0 Hz, 1H), 7.48-7.52 (m, 2H), 7.70 (d, *J* = 2.0 Hz, 1H), 7.73-7.77 (m, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 8.32 (dd, *J* = 8.0 Hz, 1.2 Hz, 1H) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 118.2, 120.8, 121.2, 121.9, 124.5, 126.9, 127.7, 128.3 129.4, 135.3, 156.1, 156.3, 176.7 ppm. HRMS (ESI⁺): calcd for C₁₃H₈⁷⁹BrO₂ [M+H]⁺ 274.9702, found 274.9708, calcd for C₁₃H₈⁸¹BrO₂ [M+H]⁺ 276.9682, found 276.9683.

3-(4-(9,9-Dimethylacridin-10(9H)-yl)phenyl)-9H-xanthen-9-one (ACRXTO). H₂O (1.2 mL) and THF (4.8 mL) were added to a mixture of 3-bromo-9H-xanthen-9-one (658 mg, 2.4 mmol), (4-(9,9-dimethylacridin-10(9H)-yl)phenyl)boronic acid (1.0 g, 3.2 mmol), Na₂CO₃ (508 mg, 4.8 mmol) and Pd(PPh₃)₄ (140 mg, 0.12 mmol) under a N₂ atmosphere. The reaction mixture was stirred at 80 °C for 12 h. The resulting solution was cooled to ambient temperature, diluted with 5 mL of dichloromethane and water, filtered and washed with 10-20 mL of petroleum ether. The obtained solid was dissolved with dichloromethane, filtered through a celite pad and washed with dichloromethane. Then the filtrate was collected, and concentrated by rotary evaporator. The crude product was further purified by recrystallization from dichloromethane to afford ACRXTO as a white solid (960 mg, 84%). ¹H NMR (400 MHz, CDCl₃): $\delta = 1.72$ (s, 6H), 6.36 (dd, J = 8.0 Hz, 1.2 Hz, 2H), 6.94-7.03 (m, 4H), 7.41-7.45 (m, 1H), 7.48-7.51 (m, 4H), 7.56 (d, J = 7.6 Hz, 1H), 7.73-7.78 (m, 2H), 7.83 (d, J = 1.6 Hz, 1H), 7.97 (dt, J = 8.8 Hz, 2.0 Hz, 2H), 8.39 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 8.47 (d, J = 8.4 Hz, 1H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 31.4$, 36.1, 114.1, 116.3, 118.2, 120.9, 121.0, 122.2, 123.2, 124.2, 125.5, 126.6, 126.9, 127.6, 130.0, 130.2, 132.2, 135.1, 139.2, 140.9, 141.9, 147.0, 156.5, 156.7, 177.1 ppm. HRMS (ESI⁺): calcd for C₃₄H₂₅NNaO₂ [M+Na]⁺ 502.1778, found 502.1776.

(ii) Synthesis of 8-MeACRXTO



6-Bromo-1-methyl-9*H***-xanthen-9-one.** Pyridine (0.4 mL, 5 mmol) and DMF (10 mL) were added to a mixture of 2-iodo-6-methylbenzoic acid (1.3 g, 5 mmol),

3-bromophenol (1.7 g, 10 mmol), copper (47.6 mg, 0.75 mmol), CuI (47.5 mg, 0.25 mmol), and K₂CO₃ (1.0 g, 7.5 mmol) under a N₂ atmosphere. The reaction mixture was stirred at 100 °C for 24 h. The resulting solution was cooled to ambient temperature, diluted with brine solution and ethyl acetate, and acidified by concentrated HCl to pH = 1. The organic extracts were washed with water, dried over Na₂SO₄ and concentrated under reduced pressure. The resulting residue was treated with triflic acid (5 mL) at 100 °C for 3 h. After that, it was allowed to cool to room temperature and quenched with water. The mixture was extracted with dichloromethane (DCM) and organic phase was separated, dried over Na₂SO₄, filtered, and evaporated under vacuum. Purification by column chromatography on silica gel (petroleum ether/ethyl acetate 60/1. v/v) afforded = 6-bromo-1-methyl-9H-xanthen-9-one as a white solid (450 mg, 31% yield). ¹H NMR (400 MHz, CDCl₃): δ = 2.91 (s, 3H), 7.14 (d, J = 7.2 Hz, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.46 (dd, J = 8.4 Hz, 1.6 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.63 (d, J = 1.6 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 23.4$, 116.2, 120.3, 120.7, 121.8, 127.3, 127.5, 128.3, 128.8, 134.2, 142.4, 155.5, 157.6, 178.4 ppm. HRMS (ESI⁺): calcd for C₁₄H₉⁷⁹BrNaO₂ [M+Na]⁺ 310.9678, found 310.9680, calcd for C₁₄H₉⁸¹BrNaO₂ [M+Na]⁺ 312.9658, found 312.9657.

6-(4-(9,9-Dimethylacridin-10(9H)-yl)phenyl)-1-methyl-9H-xanthen-9-one

(8-MeACRXTO). H₂O (1.2 mL) and THF (4.8 mL) were added to a mixture of 6-bromo-1-methyl-9*H*-xanthen-9-one (691 mg, 2.4 mmol), (4-(9,9-dimethylacridin-10(9H)-yl)phenyl)boronic acid (1.0 g, 3.2 mmol), Na₂CO₃ (508 mg, 4.8 mmol) and Pd(PPh₃)₄ (140 mg, 0.12 mmol) under a N₂ atmosphere. The reaction mixture was stirred at 80 °C for 12 h. The resulting solution was cooled to ambient temperature, diluted with 5 mL of dichloromethane and water, filtered and washed with 10-20 mL of petroleum ether. The obtained solid was dissolved with dichloromethane, filtered through a celite pad and washed with dichloromethane. Then the filtrate was collected, and concentrated by rotary evaporator. The crude product was further purified by recrystallization from dichloromethane to afford **8-MeACRXTO** as a white solid (1040 mg, 88%). ¹H NMR (400 MHz, CDCl₃): $\delta =$ 1.72 (s, 6H), 2.98 (s, 3H), 6.35 (dd, J = 8.0 Hz, 1.2 Hz, 2H), 6.93-7.03 (m, 4H), 7.16 (d, J = 7.6 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.47-7.49 (m, 4H), 7.59 (t, J = 7.6 Hz, 1H), 7.70 (dd, *J* = 8.4 Hz, 1.6 Hz, 1H), 7.77 (d, *J* = 1.6 Hz, 1H), 7.96 (dt, *J* = 8.8 Hz, 2.0 Hz, 2H), 8.40 (d, J = 8.0 Hz, 1H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 23.5$, 31.4, 36.1, 114.2, 115.8, 116.2, 120.6, 120.9, 122.0, 123.0, 125.5, 126.5, 127.0, 127.6, 130.0, 130.2, 132.1, 134.0, 139.3, 140.9, 141.8, 146.5, 155.8, 157.9, 178.9 ppm. HRMS (ESI⁺): calcd for C₃₅H₂₇NNaO₂ [M+Na]⁺ 516.1934, found 516.1940.

(iii) Synthesis of 1-MeACRXTO



3-Bromo-1-methyl-9H-xanthen-9-one. Pyridine (0.4 mL, 5 mmol) and DMF (10 mL) were added to a mixture of 4-bromo-2-iodo-6-methylbenzoic acid (1.7 g, 5 mmol), phenol (940 mg, 10 mmol), copper (47.6 mg, 0.75 mmol), CuI (47.5 mg, 0.25 mmol), and K₂CO₃ (1.0 g, 7.5 mmol) under a N₂ atmosphere. The reaction mixture was stirred at 100 °C for 24 h. The resulting solution was cooled to ambient temperature, diluted with brine solution and ethyl acetate, and acidified by concentrated HCl to pH = 1. The organic extracts were washed with water, dried over Na₂SO₄ and concentrated under reduced pressure. The resulting residue was treated with triflic acid (5 mL) at 100 °C for 3 h. After that, it was allowed to cool to room temperature and quenched with water. The mixture was extracted with dichloromethane (DCM) and organic phase was separated, dried over Na₂SO₄, filtered, and evaporated under vacuum. Purification by column chromatography silica on gel (petroleum ether/dichloromethane = 5/1, v/v) afforded **3-bromo-1-methyl-9H-xanthen-9-one** as a white solid (700 mg, 49% yield). ¹H NMR (400 MHz, CDCl₃): $\delta = 2.90$ (s, 3H), 7.26-7.27 (overlap, 1H), 7.37 (t, J = 8.0 Hz, 1H), 7.42 (d, J = 8.4 Hz, 1H), 7.53 (s, 1H), 7.68-7.72 (m, 1H), 8.26 (dd, J = 8.0 Hz, 1.6 Hz, 1H) ppm. ¹³C NMR (100 MHz, $CDCl_3$): $\delta = 23.3, 117.6, 119.3, 122.8, 124.3, 126.8, 127.9, 130.0, 134.8, 144.0, 155.2, 126.8, 127.9, 130.0, 134.8, 144.0, 155.2, 126.8, 126.8, 127.9, 130.0, 134.8, 144.0, 155.2, 126.8,$ 157.6, 178.4 ppm. HRMS (ESI⁺): calcd for C₁₄H₁₀⁷⁹BrO₂ [M+H]⁺ 288.9859, found 288.9858, calcd for $C_{14}H_{10}^{81}BrO_2 [M+H]^+$ 290.9838, found 290.9838.

3-(4-(9,9-Dimethylacridin-10(9H)-yl)phenyl)-1-methyl-9H-xanthen-9-one

(1-MeACRXTO). H₂O (1.2 mL) and THF (4.8 mL) were added to a mixture of 3-bromo-1-methyl-9*H*-xanthen-9-one (691 2.4mg, mmol). (4-(9,9-dimethylacridin-10(9H)-yl)phenyl)boronic acid (1.0 g, 3.2 mmol), Na₂CO₃ (508 mg, 4.8 mmol) and Pd(PPh₃)₄ (140 mg, 0.12 mmol) under a N₂ atmosphere. The reaction mixture was stirred at 80 °C for 12 h. The resulting solution was cooled to ambient temperature, diluted with 5 mL of dichloromethane and water, filtered and washed with 10-20 mL of petroleum ether. The obtained solid was dissolved with dichloromethane, filtered through a celite pad and washed with dichloromethane. Then the filtrate was collected, and concentrated by rotary evaporator. The crude product was further purified by recrystallization from dichloromethane to afford **1-MeACRXTO** as a white solid (720 mg, 61%). ¹H NMR (400 MHz, CDCl₃): $\delta =$ 1.72 (s, 6H), 3.05 (s, 3H), 6.35 (d, J = 7.2 Hz, 2H), 6.93-7.03 (m, 4H), 7.37-7.41 (m, 1H), 7.46-7.50 (m, 6H), 7.67 (d, J = 1.6 Hz, 1H), 7.70-7.74 (m, 1H), 7.96 (dt, J = 8.4 Hz, 2.4 Hz, 2H), 8.32 (dd, J = 8.0 Hz, 1.6 Hz, 1H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 23.8, 31.4, 36.1, 114.2, 114.4, 117.6, 119.5, 120.9, 123.1, 124.0, 125.5, 125.8,$ 126.5, 126.9, 130.0, 130.2, 132.1, 134.6, 139.1, 140.9, 141.8, 142.9, 145.5, 155.6,

158.1, 178.8 ppm. HRMS (ESI⁺): calcd for $C_{35}H_{27}NNaO_2 [M+Na]^+$ 516.1934, found 516.1936.

(iv) Synthesis of *d*MeACRXTO



3-Bromo-1,8-dimethyl-9H-xanthen-9-one. Pyridine (0.4 mL, 5 mmol) and DMF (10 mL) were added to a mixture of 4-bromo-2-iodo-6-methylbenzoic acid (1.7 g, 5 mmol), *m*-cresol (1.1 g, 10 mmol), copper (47.6 mg, 0.75 mmol), CuI (47.5 mg, 0.25 mmol), and K_2CO_3 (1.0 g, 7.5 mmol) under a N_2 atmosphere. The reaction mixture was stirred at 100 °C for 24 h. The resulting solution was cooled to ambient temperature, diluted with brine solution and ethyl acetate, and acidified by concentrated HCl to pH = 1. The organic extracts were washed with water, dried over Na₂SO₄ and concentrated under reduced pressure. The resulting residue was treated with triflic acid (5 mL) at 100 °C for 3 h. After that, it was allowed to cool to room temperature and quenched with water. The mixture was extracted with dichloromethane (DCM) and organic phase was separated, dried over Na₂SO₄, filtered, and evaporated under vacuum. Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 60/1. v/v) afforded **3-bromo-1,8-dimethyl-9H-xanthen-9-one** as a white solid (300 mg, 20% yield). ¹H NMR (400 MHz, CDCl₃): $\delta = 2.84$ (s, 3H), 2.86 (s, 3H), 7.08 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 0.8 Hz, 1H), 7.23 (d, J = 8.4 Hz, 1H), 7.44 (d, J = 1.6 Hz, 1H), 7.50 (t, J = 8.0 Hz)Hz, 1H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 23.3, 23.4, 115.7, 118.8, 120.3, 121.4,$ 127.1, 127.2, 129.8, 133.6, 141.9, 143.6, 156.5, 156.8, 180.5 ppm. HRMS (ESI⁺): calcd for $C_{15}H_{12}^{79}BrO_2 [M+H]^+$ 303.0015, found 303.0015, calcd for $C_{15}H_{12}^{81}BrO_2$ [M+H]⁺ 304.9995, found 304.9993.

3-(4-(9,9-Dimethylacridin-10(9H)-yl)phenyl)-1,8-dimethyl-9H-xanthen-9-one

(dMeACRXTO). H₂O (0.6 mL) and THF (2.4 mL) were added to a mixture of 3-bromo-1,8-dimethyl-9H-xanthen-9-one (362 1.2 mg, mmol). (4-(9,9-dimethylacridin-10(9H)-yl)phenyl)boronic acid (500 mg, 1.6 mmol), Na₂CO₃ (254 mg, 2.4 mmol) and Pd(PPh₃)₄ (70 mg, 0.06 mmol) under a N₂ atmosphere. The reaction mixture was stirred at 80 °C for 12 h. The resulting solution was cooled to ambient temperature, diluted with 2 mL of dichloromethane and water, filtered and washed with 10-20 mL of petroleum ether. The obtained solid was dissolved with dichloromethane, filtered through a celite pad and washed with dichloromethane. Then the filtrate was collected, and concentrated by rotary evaporator. The crude product was further purified by recrystallization from dichloromethane to afford *d*MeACRXTO as a white solid (410 mg, 69%). ¹H NMR (400 MHz, CDCl₃): $\delta =$ 1.72 (s, 6H), 2.93 (s, 3H), 3.00 (s, 3H), 6.35 (d, J = 7.2 Hz, 2H), 6.93-7.03 (m, 4H),

7.12 (d, J = 7.2 Hz, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.43 (s, 1H), 7.46-7.49 (m, 4H), 7.53 (t, J = 7.6 Hz, 1H), 7.61 (d, J = 1.6 Hz, 1H), 7.95 (d, J = 8.4 Hz, 2H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 23.5$, 23.8, 31.4, 36.1, 113.9, 114.1, 115.7, 120.6, 120.8, 121.6, 125.4, 125.7, 126.5, 126.9, 129.9, 130.2, 132.0, 133.4, 139.2, 140.9, 141.7, 141.9, 142.5, 144.9, 157.0, 157.2, 180.9 ppm. HRMS (ESI⁺): calcd for C₃₆H₂₉NNaO₂ [M+Na]⁺ 530.2091, found 530.2098.

III. Crystal Data

Identification code	ACRXTO
Empirical formula	C ₃₄ H ₂₅ NO ₂
Formula weight	479.55
Temperature/K	297.90 (18)
Crystal system	monoclinic
Space group	P21/c
a/Å	9.7627 (2)
b/Å	15.2824 (3)
c/Å	17.0059 (4)
α/°	90
β/°	100.126 (2)
$\gamma/^{\circ}$	90
Volume/Å ³	2497.74 (10)
Z	4
pcalcg/cm ³	1.275
µ/mm ⁻¹	0.617
F(000)	1008.0
Crystal size/mm ³	0.5 imes 0.3 imes 0.3
Radiation	$CuK\alpha \ (\lambda = 1.54184)$
2Θ range for data collection/°	7.834 to 143.118
Index ranges	$-11 \le h \le 9, -18 \le k \le 18, -19 \le l \le 20$
Reflections collected	13838
Independent reflections	4795 [$R_{int} = 0.0374$, $R_{sigma} = 0.0337$]
Data/restraints/parameters	4795/0/336
Goodness-of-fit on F ²	1.035
Final R indexes [I>= 2σ (I)]	$R_1 = 0.0592, wR_2 = 0.1609$
Final R indexes [all data]	$R_1 = 0.0694, wR_2 = 0.1763$
Largest diff. peak/hole / e Å ⁻³	0.19/-0.31

Table S1. Crystal Data for ACRXTO

Table S2.	Crystal	Data :	for 8-	-MeA	CRXT	0
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Identification code	8-MeACRXTO
Empirical formula	C ₃₅ H ₂₇ NO ₂

Formula weight	493.57
Temperature/K	296.82 (11)
Crystal system	monoclinic
Space group	P21/c
a/Å	9.25345 (19)
b/Å	34.5061 (6)
c/Å	8.13039 (16)
$\alpha/^{\circ}$	90
β/°	106.251 (2)
γ/°	90
Volume/Å ³	2492.31 (9)
Z	4
pcalcg/cm ³	1.315
µ/mm ⁻¹	0.633
F(000)	1040.0
Crystal size/mm ³	0.6 imes 0.35 imes 0.25
Radiation	$CuK\alpha$ ($\lambda = 1.54184$)
2Θ range for data collection/°	9.956 to 142.932
Index ranges	$-10 \le h \le 11, -42 \le k \le 35, -9 \le l \le 8$
Reflections collected	13748
Independent reflections	4765 $[R_{int} = 0.0442, R_{sigma} = 0.0329]$
Data/restraints/parameters	4765/0/346
Goodness-of-fit on F ²	1.054
Final R indexes [I>=2σ (I)]	$R_1 = 0.0623, wR_2 = 0.1669$
Final R indexes [all data]	$R_1 = 0.0694, wR_2 = 0.1755$
Largest diff. peak/hole / e Å ⁻³	0.26/-0.27

Table S3. Crystal Data for 1-MeACRXTO

Identification code	1-MeACRXTO
Empirical formula	C ₃₅ H ₂₇ NO ₂
Formula weight	493.57
Temperature/K	150.01 (10)
Crystal system	triclinic
Space group	P-1
a/Å	9.2312 (5)
b/Å	10.2169 (7)
c/Å	14.6844 (8)
$\alpha /^{\circ}$	76.439 (5)
β/°	87.971 (5)
$\gamma/^{\circ}$	67.260 (6)
Volume/Å ³	1239.33 (14)
Z	2
pcalcg/cm ³	1.323

μ/mm^{-1}	0.637
F(000)	520.0
Crystal size/mm ³	0.25 imes 0.15 imes 0.1
Radiation	$CuK\alpha \ (\lambda = 1.54184)$
2Θ range for data collection/°	9.668 to 143.002
Index ranges	$-9 \le h \le 11, -12 \le k \le 12, -11 \le l \le 17$
Reflections collected	9294
Independent reflections	$4641 \ [R_{int} = 0.0369, R_{sigma} = 0.0482]$
Data/restraints/parameters	4641/0/346
Goodness-of-fit on F ²	1.040
Final R indexes [I>=2σ (I)]	$R_1 = 0.0584, wR_2 = 0.1517$
Final R indexes [all data]	$R_1 = 0.0696, wR_2 = 0.1664$
Largest diff. peak/hole / e Å ⁻³	0.36/-0.33

Table S4. Crystal Data for dMeACRXTO

Identification code $dMeACRXTO$ Empirical formula $C_{36}H_{29}NO_2$ Formula weight 507.60 Temperature/K 293.15 Crystal system triclinic Space group P-1 $a/Å$ 9.6146 (5) $b/Å$ 16.2601 (8) $c/Å$ 18.3252 (9) a'° 110.783 (5) β'° 90.710 (4) γ'° 101.904 (4) Volume/Å ³ 2609.3 (2) Z 4 pcalcg/cm ³ 1.292 μ/mm^{-1} 0.079 F(000) 1072.0 Crystal size/mm ³ 0.3 × 0.2 × 0.05 Radiation MoK α ($\lambda = 0.71073$) 2 Θ range for data collection/° 5.646 to 52.744 Index ranges -12 ≤ h ≤ 12, -20 ≤ k ≤ 19, -22 ≤ 1 ≤ 22 Reflections collected 20543 Independent reflections 10638 [Rimt = 0.0494, R_{sigma} = 0.1497] Data/restraints/parameters 10638/0/711 Goodness-of-fit on F ² 0.939 Final R indexes		
Empirical formula $C_{36}H_{29}NO_2$ Formula weight 507.60 Temperature/K 293.15 Crystal system triclinic Space group P-1 $a/Å$ 9.6146 (5) $b/Å$ 16.2601 (8) $c/Å$ 18.3252 (9) a'° 110.783 (5) $\beta/^\circ$ 90.710 (4) γ'° 101.904 (4) Volume/Å ³ 2609.3 (2) Z 4 pcalcg/cm ³ 1.292 μ/mm^{-1} 0.079 F(000) 1072.0 Crystal size/mm ³ 0.3 × 0.2 × 0.05 Radiation MoKa ($\lambda = 0.71073$) 2 Θ range for data collection/° 5.646 to 52.744 Index ranges -12 ≤ h ≤ 12, -20 ≤ k ≤ 19, -22 ≤ l ≤ 22 Reflections collected 20543 Independent reflections 10638 [R _{int} = 0.0494, R _{sigma} = 0.1497] Data/restraints/parameters 10638/0/711 Goodness-of-fit on F ² 0.939 Final R indexes [I] data] R ₁ = 0.2122, wR ₂ = 0.1038 <td< td=""><td>Identification code</td><td>dMeACRXTO</td></td<>	Identification code	dMeACRXTO
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$ b/Å \qquad 16.2601 (8) \\ c/Å \qquad 18.3252 (9) \\ \alpha/^{\circ} \qquad 110.783 (5) \\ \beta/^{\circ} \qquad 90.710 (4) \\ \gamma/^{\circ} \qquad 101.904 (4) \\ Volume/Å^{3} \qquad 2609.3 (2) \\ Z \qquad 4 \\ \rho calcg/cm^{3} \qquad 1.292 \\ \mu/mm^{-1} \qquad 0.079 \\ F(000) \qquad 1072.0 \\ Crystal size/mm^{3} \qquad 0.3 \times 0.2 \times 0.05 \\ Radiation \qquad MoK\alpha (\lambda = 0.71073) \\ 2\Theta range for data collection/^{\circ} \qquad 5.646 to 52.744 \\ Index ranges \qquad -12 \le h \le 12, -20 \le k \le 19, -22 \le 1 \le 22 \\ Reflections collected \qquad 20543 \\ Independent reflections \qquad 10638 [R_{int} = 0.0494, R_{sigma} = 0.1497] \\ Data/restraints/parameters \qquad 10638/0/711 \\ Goodness-of-fit on F^{2} \qquad 0.939 \\ Final R indexes [I>=2\sigma (I)] \qquad R_{1} = 0.0656, wR_{2} = 0.1038 \\ Final R indexes [all data] \qquad R_{1} = 0.2122, wR_{2} = 0.1542 \\ Largest diff. peak/hole / e Å^{z3} \qquad 0.17/-0.19 \\ $	a/Å	9.6146 (5)
$\begin{array}{lll} c/ \mathring{A} & & 18.3252 \ (9) \\ a/^{\circ} & & 110.783 \ (5) \\ \beta/^{\circ} & & 90.710 \ (4) \\ \gamma/^{\circ} & & 101.904 \ (4) \\ \mbox{Volume}/ \mathring{A}^3 & & 2609.3 \ (2) \\ Z & & 4 \\ \mbox{pcalcg/cm}^3 & & 1.292 \\ \mu/mm^{-1} & & 0.079 \\ F(000) & & 1072.0 \\ \mbox{Crystal size/mm}^3 & & 0.3 \times 0.2 \times 0.05 \\ \mbox{Radiation} & & MoK\alpha \ (\lambda = 0.71073) \\ 2\Theta \ range \ for \ data \ collection/^{\circ} & 5.646 \ to \ 52.744 \\ \mbox{Index ranges} & -12 \le h \le 12, -20 \le k \le 19, -22 \le l \le 22 \\ \mbox{Reflections \ collected} & & 20543 \\ \mbox{Independent \ reflections} & & 10638 \ [R_{int} = 0.0494, R_{sigma} = 0.1497] \\ \mbox{Data/restraints/parameters} & & 10638/0/711 \\ \mbox{Goodness-of-fit on \ F}^2 & 0.939 \\ \mbox{Final \ R \ indexes \ [l>=2\sigma \ (l)]} & R_1 = 0.0656, \ wR_2 = 0.1038 \\ \mbox{Final \ R \ indexes \ [all \ data]} & R_1 = 0.2122, \ wR_2 = 0.1542 \\ \mbox{Largest \ diff. peak/hole / e \ \mathring{A}^{-3}} & 0.17/-0.19 \\ \end{array}$	b/Å	16.2601 (8)
$\begin{array}{lll} \mathfrak{a}/^{\circ} & 110.783 (5) \\ \mathfrak{\beta}/^{\circ} & 90.710 (4) \\ \mathfrak{\gamma}/^{\circ} & 101.904 (4) \\ \mbox{Volume/Å}^3 & 2609.3 (2) \\ \mbox{Z} & 4 \\ \mbox{ρcalcg/cm}^3 & 1.292 \\ \mu/mm^{-1} & 0.079 \\ \mbox{$F(000)$} & 1072.0 \\ \mbox{$Crystal size/mm}^3 & 0.3 \times 0.2 \times 0.05 \\ \mbox{$Radiation$} & MoK\alpha (\lambda = 0.71073) \\ \mbox{2Θ} range for data collection/^{\circ} & 5.646 to 52.744 \\ \mbox{$Index ranges$} & -12 \le h \le 12, -20 \le k \le 19, -22 \le l \le 22 \\ \mbox{$Reflections collected$} & 20543 \\ \mbox{$Independent reflections$} & 10638 [R_{int} = 0.0494, R_{sigma} = 0.1497] \\ \mbox{$Data/restraints/parameters$} & 10638/0/711 \\ \mbox{$Godness-of-fit on F^2} & 0.939 \\ \mbox{$Final R indexes $[I>=2\sigma$ (I)]$} & R_1 = 0.0656, wR_2 = 0.1038 \\ \mbox{$Final R indexes $[all data]$} & R_1 = 0.2122, wR_2 = 0.1542 \\ \mbox{$Largest diff. peak/hole / e $$A}^{-3}$} & 0.17/-0.19 \\ \end{array}$	c/Å	18.3252 (9)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$\alpha/^{\circ}$	110.783 (5)
$\begin{array}{lll} \gamma /^{\circ} & 101.904 \ (4) \\ \mbox{Volume/Å}^3 & 2609.3 \ (2) \\ \mbox{Z} & 4 \\ \mbox{ρcalcg/cm}^3 & 1.292 \\ \mbox{$\mu/mm}^{-1$} & 0.079 \\ \mbox{$F(000)$} & 1072.0 \\ \mbox{$Crystal size/mm}^3 & 0.3 \times 0.2 \times 0.05 \\ \mbox{$Radiation$} & MoK\alpha \ (\lambda = 0.71073) \\ \mbox{2Θ range for data collection/$^{\circ}$} & 5.646 \ to \ 52.744 \\ \mbox{$Index ranges$} & -12 \le h \le 12, -20 \le k \le 19, -22 \le l \le 22 \\ \mbox{$Reflections collected$} & 20543 \\ \mbox{$Independent reflections$} & 10638 \ [R_{int} = 0.0494, R_{sigma} = 0.1497] \\ \mbox{$Data/restraints/parameters$} & 10638/0/711 \\ \mbox{$Goodness-of-fit on F^2} & 0.939 \\ \mbox{$Final R indexes $[I>=2\sigma$ (I)]$} & R_1 = 0.0656, \ wR_2 = 0.1038 \\ \mbox{$Final R indexes $[all data]$} & R_1 = 0.2122, \ wR_2 = 0.1542 \\ \mbox{$Largest diff. peak/hole $/ e$ $ $Å^{-3}$} & 0.17/-0.19 \\ \end{array}$	β/°	90.710 (4)
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$\begin{array}{llllllllllllllllllllllllllllllllllll$	Volume/Å ³	2609.3 (2)
$\begin{array}{lll} \mbox{ρcalcg/cm}^3$ & 1.292 \\ \mbox{μ/mm^{-1}} & 0.079 \\ \mbox{$F(000)$} & 1072.0 \\ \mbox{Crystal size/mm}^3$ & 0.3 \times 0.2 \times 0.05 \\ \mbox{$Radiation$} & MoK\alpha~(\lambda=0.71073) \\ \mbox{2Θ range for data collection/$^{\circ}$} & 5.646 to 52.744 \\ \mbox{$Index ranges$} & -12 \le h \le 12, -20 \le k \le 19, -22 \le 1 \le 22 \\ \mbox{$Reflections collected$} & 20543 \\ \mbox{$Independent reflections$} & 10638~[R_{int}=0.0494, R_{sigma}=0.1497] \\ \mbox{$Data/restraints/parameters$} & 10638/0/711 \\ \mbox{$Goodness-of-fit on F}^2$ & 0.939 \\ \mbox{$Final R indexes [I]=2\sigma~(I)]$} & R_1 = 0.0656, wR_2 = 0.1038 \\ \mbox{$Final R indexes [all data]$} & R_1 = 0.2122, wR_2 = 0.1542 \\ \mbox{$Largest diff. peak/hole / e Å}^{-3}$ & 0.17/-0.19 \\ \end{array}$	Z	4
$\begin{array}{lll} \mu/mm^{-1} & 0.079 \\ F(000) & 1072.0 \\ Crystal size/mm^3 & 0.3 \times 0.2 \times 0.05 \\ Radiation & MoK\alpha (\lambda = 0.71073) \\ 2\Theta \ range for data collection/^{\circ} & 5.646 \ to \ 52.744 \\ Index \ ranges & -12 \leq h \leq 12, -20 \leq k \leq 19, -22 \leq l \leq 22 \\ Reflections collected & 20543 \\ Independent \ reflections & 10638 \ [R_{int} = 0.0494, \ R_{sigma} = 0.1497] \\ Data/restraints/parameters & 10638/0/711 \\ Goodness-of-fit \ on \ F^2 & 0.939 \\ Final \ R \ indexes \ [I>=2\sigma \ (I)] & R_1 = 0.0656, \ wR_2 = 0.1038 \\ Final \ R \ indexes \ [all \ data] & R_1 = 0.2122, \ wR_2 = 0.1542 \\ Largest \ diff. \ peak/hole \ / \ e \ Å^{-3} & 0.17/-0.19 \\ \end{array}$	pcalcg/cm ³	1.292
$\begin{array}{lll} F(000) & 1072.0 \\ Crystal size/mm^3 & 0.3 \times 0.2 \times 0.05 \\ Radiation & MoK\alpha (\lambda = 0.71073) \\ 2\Theta \ range for data \ collection/^{\circ} & 5.646 \ to \ 52.744 \\ Index \ ranges & -12 \leq h \leq 12, \ -20 \leq k \leq 19, \ -22 \leq l \leq 22 \\ Reflections \ collected & 20543 \\ Independent \ reflections & 10638 \ [R_{int} = 0.0494, \ R_{sigma} = 0.1497] \\ Data/restraints/parameters & 10638/0/711 \\ Goodness-of-fit \ on \ F^2 & 0.939 \\ Final \ R \ indexes \ [I>=2\sigma \ (I)] & R_1 = 0.0656, \ wR_2 = 0.1038 \\ Final \ R \ indexes \ [all \ data] & R_1 = 0.2122, \ wR_2 = 0.1542 \\ Largest \ diff. \ peak/hole \ / \ e \ Å^{-3} & 0.17/-0.19 \\ \end{array}$	μ/mm^{-1}	0.079
$\begin{array}{llllllllllllllllllllllllllllllllllll$	F(000)	1072.0
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$\begin{array}{llllllllllllllllllllllllllllllllllll$	Radiation	MoKa ($\lambda = 0.71073$)
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	2Θ range for data collection/°	5.646 to 52.744
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$\begin{array}{llllllllllllllllllllllllllllllllllll$	Independent reflections	10638 [$R_{int} = 0.0494$, $R_{sigma} = 0.1497$]
Goodness-of-fit on F^2 0.939 Final R indexes [I>=2 σ (I)] $R_1 = 0.0656$, $wR_2 = 0.1038$ Final R indexes [all data] $R_1 = 0.2122$, $wR_2 = 0.1542$ Largest diff. peak/hole / e Å ⁻³ 0.17/-0.19	Data/restraints/parameters	10638/0/711
Final R indexes [I>=2 σ (I)] $R_1 = 0.0656$, $wR_2 = 0.1038$ Final R indexes [all data] $R_1 = 0.2122$, $wR_2 = 0.1542$ Largest diff. peak/hole / e Å ⁻³ $0.17/-0.19$	Goodness-of-fit on F ²	0.939
Final R indexes [all data] $R_1 = 0.2122, wR_2 = 0.1542$ Largest diff. peak/hole / e Å ⁻³ $0.17/-0.19$	Final R indexes [I>=2 σ (I)]	$R_1 = 0.0656, wR_2 = 0.1038$
Largest diff. peak/hole / e Å-3 $0.17/-0.19$	Final R indexes [all data]	$R_1 = 0.2122, wR_2 = 0.1542$
	Largest diff. peak/hole / e Å ⁻³	0.17/-0.19

IV. Theoretical calculation

Theoretical calculations were carried out using Gaussian 09 software.¹ The ground-state structures were optimized by density functional theory (DFT) at B3LYP/6-31G* level.²⁻³ The S₁ and T₁ energies were calculated by time-dependent DFT (TD-DFT) method. The electrostatic potentials and FMO distributions were visualized using Gaussview 5.0 software. The charge-transfer integrals (ν) were calculated at PW91PW91/6-31G (d, p) level based on the single crystal structures.⁴⁻⁶



Fig. S1 (a) The calculated electron-transfer integral in the horizontal packing direction of XTO plane for ACRXTO, 1-MeACRXTO, 8-MeACRXTO and *d*MeACRXTO. (b) The calculated electron-transfer integral in the vertical packing direction of XTO plane for ACRXTO, 1-MeACRXTO, 8-MeACRXTO and *d*MeACRXTO.

V. Additional spectra and data



Fig. S2 (a) The absorption spectra of ACRXTO, 8-MeACRXTO, 1-MeACRXTO and *d*MeACRXTO. (b) RTPL spectra of ACRXTO, 8-MeACRXTO, 1-MeACRXTO and *d*MeACRXTO. (c) LTPL spectra of ACRXTO, 8-MeACRXTO, 1-MeACRXTO and *d*MeACRXTO. (d) transient PL spectra of ACRXTO, 8-MeACRXTO, 1-MeACRXTO and *d*MeACRXTO.



Fig. S3 (a) The absorption spectrum of TBRb in CH₂Cl₂ and the PL spectra of ACRXTO, 8-MeACRXTO, 1-MeACRXTO and *d*MeACRXTO in neat films. (b) The absorption spectrum of TBRb in CH₂Cl₂ and the PL spectra of 20% DACT-II: ACRXTO, 8-MeACRXTO, 1-MeACRXTO or *d*MeACRXTO co-deposited films. (c) The PL spectrum of TBRb in CH₂Cl₂ and the PL spectra of 1% TBRb: 20% DACT-II: ACRXTO, 8-MeACRXTO, 1-MeACRXTO or *d*MeACRXTO ternary films. (d) The transient PL spectra of 1% TBRb: 20% DACT-II: ACRXTO, 1-MeACRXTO or *d*MeACRXTO, 8-MeACRXTO, 1-MeACRXTO fernary films. (d) The transient PL spectra of 1% TBRb: 20% DACT-II: ACRXTO, 8-MeACRXTO or *d*MeACRXTO fernary films.



Fig. S4 The molecular structures of DPEPO, NPB and BPhen.



Fig. S5 (a) The TGA thermograms recorded at a heating rate of 10 °C/min of ACRXTO, 8-MeACRXTO, 1-MeACRXTO and *d*MeACRXTO. (b) The cyclic voltammograms measured in dry dichloromethane containing 0.1 M of tetrabutylammonium hexafluorophosphate of ACRXTO, 8-MeACRXTO, 1-MeACRXTO and *d*MeACRXTO.



Fig. S6 Luminance-voltage-current density curves of TSF-OLED.

Table S5. The summary of carrier mobilities for ACRXTO, 8-MeACRXTO,1-MeACRXTO and dMeACRXTO.

Compound	$\mu_{ m hole} [m cm^2 V^{-1} s^{-1}]$	$\mu_{\text{electron}} \left[\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1} \right]$
ACRXTO	3.3×10^{-5}	7.1×10^{-6}
8-MeACRXTO	1.1×10^{-5}	7.2×10^{-6}
1-MeACRXTO	6.0×10^{-6}	7.7×10^{-6}
dMeACRXTO	7.9×10^{-6}	7.2×10^{-6}

VI. References

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