

## *Supporting information*

### **Tailoring the substituted position for high-efficiency charge transport ability and strong blue solid-state emission in naphthalene derivative**

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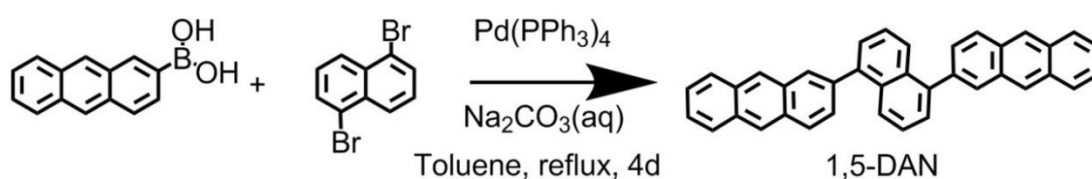
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# 1. Experiment

## 1.1 Material synthesis and characterizations

All original materials, including anthracen-2-ylboronic acid and 1,5-dibromonaphthalene, used in the synthetic route, were bought from 3A company and used without further purification. The materials synthesis of 1,5-DAN: 1 g (3.5 mmol) of 1,5-dibromonaphthalene, 1.71 g (7.69 mmol) of anthracen-2-ylboronic acid, and 202.05 mg (174.85  $\mu\text{mol}$ ) of  $\text{Pd}(\text{PPh}_3)_4$  were mixed together and added to a 250 mL flask; then the system was vacuumed and filled with argon and the process was repeated three times. Fifty milliliters of toluene and 15 mL  $\text{K}_2\text{CO}_3$  with concentration of 2 mol/L were added, and then were heated at 90 °C and stirred for 4 days. Subsequently, the system was filtered, washed with tri-ethylamine, water, methylene chloride and ethanol, and purified with a tube furnace. Finally, 1,5-DAN was obtained as a canary yellow powder with a yield of 80% or so (1.37 g).  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ , 398K)  $\delta$  8.64 (d,  $J = 7.3$  Hz, 4H), 8.22 (d,  $J = 8.7$  Hz, 2H), 8.20 (s, 2H), 8.12 – 8.08 (m, 4H), 7.96 (d,  $J = 8.3$  Hz, 2H), 7.66 (d,  $J = 8.7$  Hz, 2H), 7.60 (dt,  $J = 15.4, 7.2$  Hz, 4H), 7.53 – 7.51 (m, 4H) (Fig. S1). MS (EI)  $m/z$ : 480 [ $\text{M}^+$ ]; Anal calculated for  $\text{C}_{38}\text{H}_{24}$ : C: 94.97%, H: 5.03%. Experimental: C: 94.99%, H: 5.00%. The target compounds were characterized using elemental analysis and high-resolution mass spectroscopy, and it matched well with the final data.



Scheme S1. Synthetic route to generate 1,5-DAN.

The UV–Vis spectra were measured with Hitachi (model U-3600) UV-Vis spectrophotometer. Photoluminescence (PL) spectra data were obtained from HITACHI F-7000 spectrofluorometer. Thermal gravimetric analysis (TGA) data were obtained from a TGA 2 apparatus and the heating rate was 10 °C/min. Absolute quantum yield measurement (LabSphereR, FluoroMax4, HORIBA JobinYvon, PLQY

software package) was used for crystalline powder sample. Thin film X-ray diffraction (XRD) was measured at a voltage of 45 kV and a current of 200 mA in the reflection mode using Cu K $\alpha$  radiation by a SmartLab9KW X-ray diffractometer. Crystal X-ray diffraction data were collected at 150 K on an XtaLAB SuperNova with Cu K $\alpha$  radiation. Absolute fluorescence quantum efficiency data were obtained using a powder sample. Ultraviolet photoelectron spectroscopy (UPS) (KRATOS Axis Ultra DLD spectrometer) data were obtained using He I ( $h\nu = 21.22$  eV) as the excitation source with a base pressure  $> 2 \times 10^{-9}$  torr. Atomic force microscopy (AFM) images were obtained by using a Digital Instruments Nano-scope III atomic force microscope in air. Photoluminescence mapping were recorded at room temperature using a micro-Raman spectrometer (Renishaw, Invia microscope) with a 325 nm laser. Transmission electron microscopy (TEM) and selected area electron diffraction (SAED) were conducted on microcrystals transferred to a copper grid with a TECNAI T20 electron microscope (FEI, USA) at a low acceleration of 120 KV. OFET characteristics were recorded by a Keithley 4200 SCS and Cascade M150 probe station in an atmospheric environment.

## **1.2 OFETs preparations and measurements**

Top-contact bottom-gate organic field effect transistors of 1,5-DAN were prepared as follows. (1) The silica substrates containing 300 nm-thick SiO<sub>2</sub> layers were successively washed with deionized water, piranha solution (H<sub>2</sub>SO<sub>4</sub>/H<sub>2</sub>O<sub>2</sub> = 70/30 v/v), acetone and isopropanol, and cleaned with oxygen plasma (10 min, 80 W). (2) The cleaned silica substrates were modified with octadecyltrichlorosilane (OTS). The specific operation is as follows: First, silica substrates were dried at 90 °C (for 1.5 h) under vacuum conditions; then, a drop of OTS was added and the temperature increased to 120 °C (for 2 h) under vacuum conditions; next, the substrates were washed successively with n-hexane, trichloromethane, and isopropanol after the silica substrate cooled to room temperature. (3) Single crystals of 1,5-DAN used for organic field-effect transistors were obtained by sublimation of the sample with a two-zone tube furnace. 1,5-DAN powder as raw material was placed in the first zone (245 °C)

while the substrates were placed in the low-temperature zone. The whole system was maintained in a vacuum of 17 Pa and an argon flow rate of 30 sccm. After heating for 3 h, crystals grown on the substrate in the low-temperature zone were obtained. (4) A gold layer was obtained by sublimating gold particles under vacuum conditions on a masked substrate. The gold layer was attached on to an individual single crystal as the source or /drain electrode for the charge transport investigation using the probe. (5) The transfer and output curves of the devices were obtained at room temperature in the air with Keithley 4200 SCS and micromanipulator M150 probe station. By using of the following equation:  $I_{DS} = (W/2L) C_i \mu (V_G - V_T)^2$ , mobility was measured from the saturation region.

## 2. Figures and tables

Table S1. Crystal data and structure refinement for 1,5-DAN.

Empirical formula	C <sub>38</sub> H <sub>24</sub>
Formula weight	480.57
Temperature/K	293(2)
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 22.1427(6) Å     α = 90° b = 6.21768(16) Å     β = 91.244(3)° c = 8.9468(2) Å     γ = 90°
Volume/Å <sup>3</sup>	1231.47(6)
Z	2
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.296
μ/mm <sup>-1</sup>	0.557
F(000)	504.0
Crystal size/mm <sup>3</sup>	0.1 × 0.08 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	7.988 to 133.03
Index ranges	-26 ≤ h ≤ 26, -7 ≤ k ≤ 7, -7 ≤ l ≤ 10
Reflections collected	7224
Independent reflections	2182 [R <sub>int</sub> = 0.0175, R <sub>sigma</sub> = 0.0159]
Data/restraints/parameters	2182/0/173
Goodness-of-fit on F <sup>2</sup>	1.049
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0344, wR <sub>2</sub> = 0.0935
Final R indexes [all data]	R <sub>1</sub> = 0.0395, wR <sub>2</sub> = 0.0999
Largest diff. peak/hole / e Å <sup>-3</sup>	0.18/-0.16
CCDC number	1891732

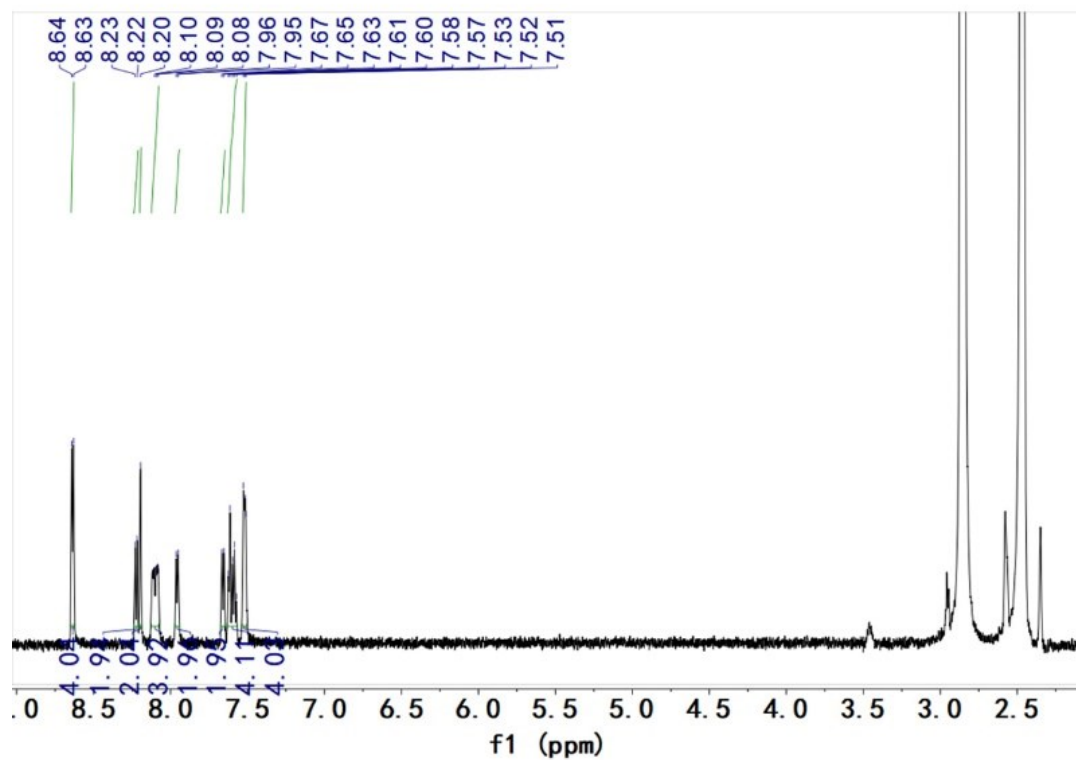


Figure S1. The  $^1\text{H}$  NMR spectrum of 1,5-DAN. (600 MHz,  $\text{DMSO-}d_6$ , 398K)

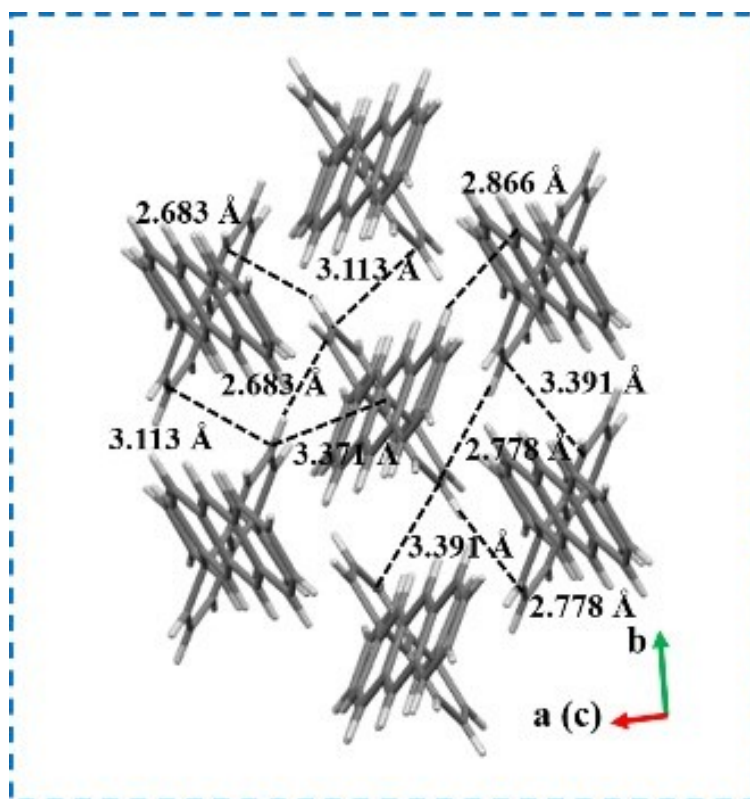


Figure S2. The short contacts and intermolecular interactions within the crystal of 1,5-DAN along different directions.

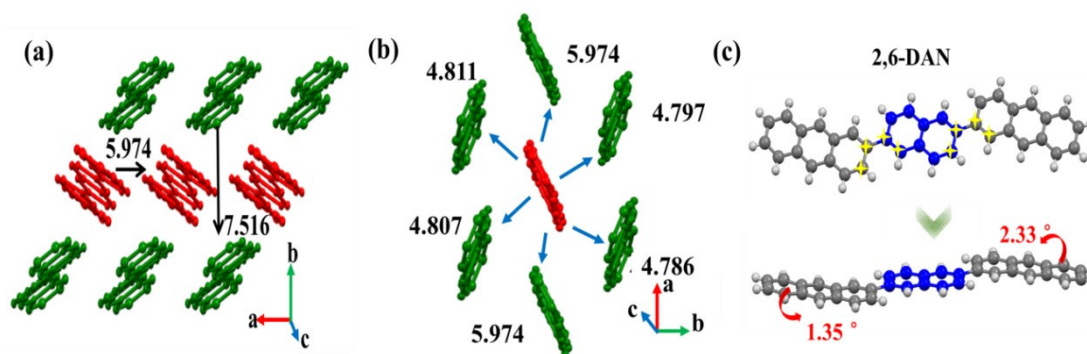


Figure S3. (a) Herringbone packing of 2,6-DAN. (b) Distance of 2,6-DAN from the surrounding molecules. (c) The views of 2,6-DAN molecule seeing perpendicular (top) to and along (side) the conjugated plane of naphthalene core. (CCDC number 1848450)

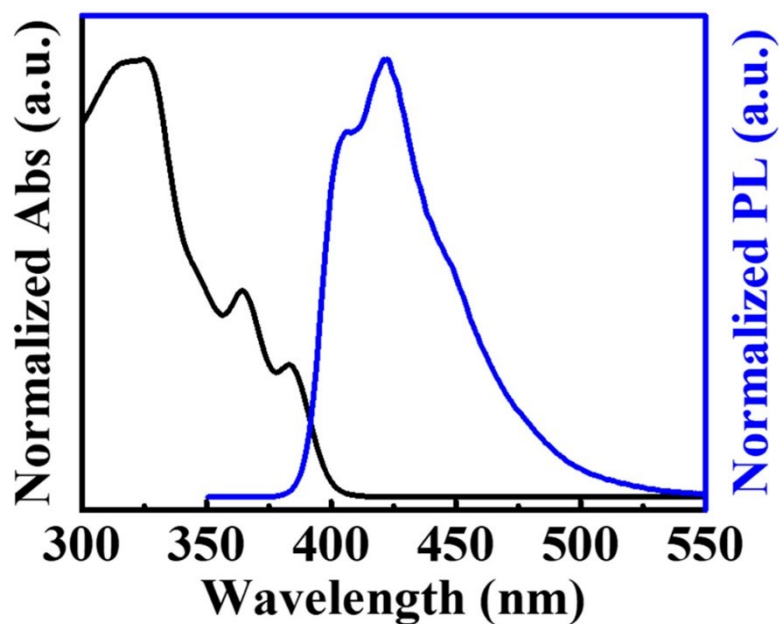


Figure S4. UV-vis absorption spectra and photoluminescence spectra of 1,5-DAN in  $C_6H_5Cl$  solutions.

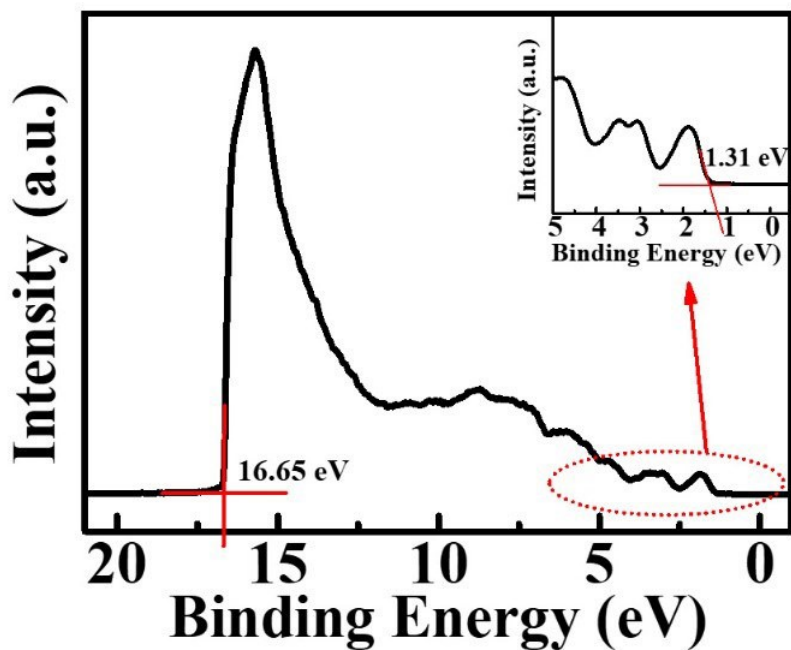


Figure S5. Ultraviolet photoelectron spectroscopy (UPS) energy distribution curve of 1,5-DAN.

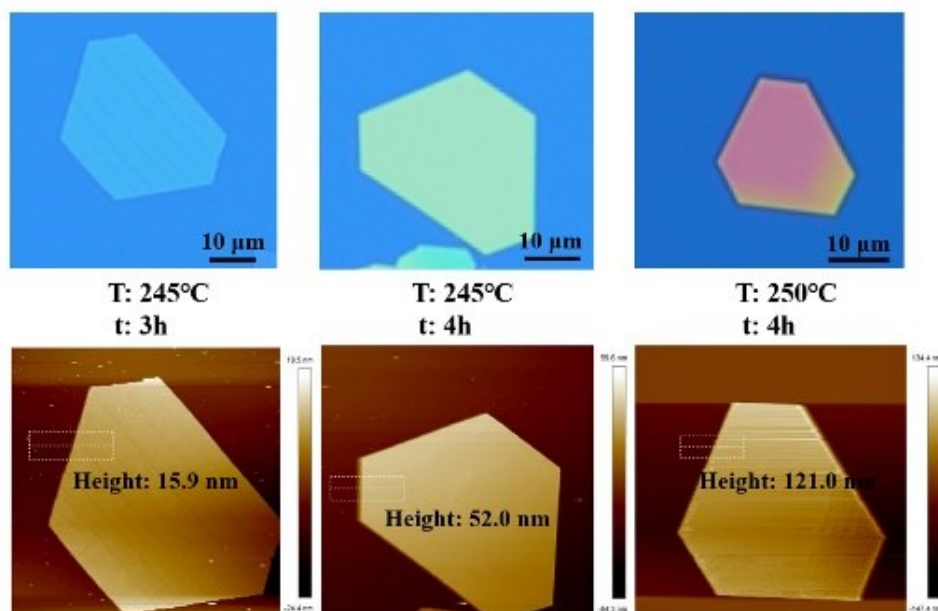


Figure S6. Optical micrographs and its corresponding atomic force microscopy (AFM) images of 1,5-DAN single crystal in different temperature (T) and time (t).



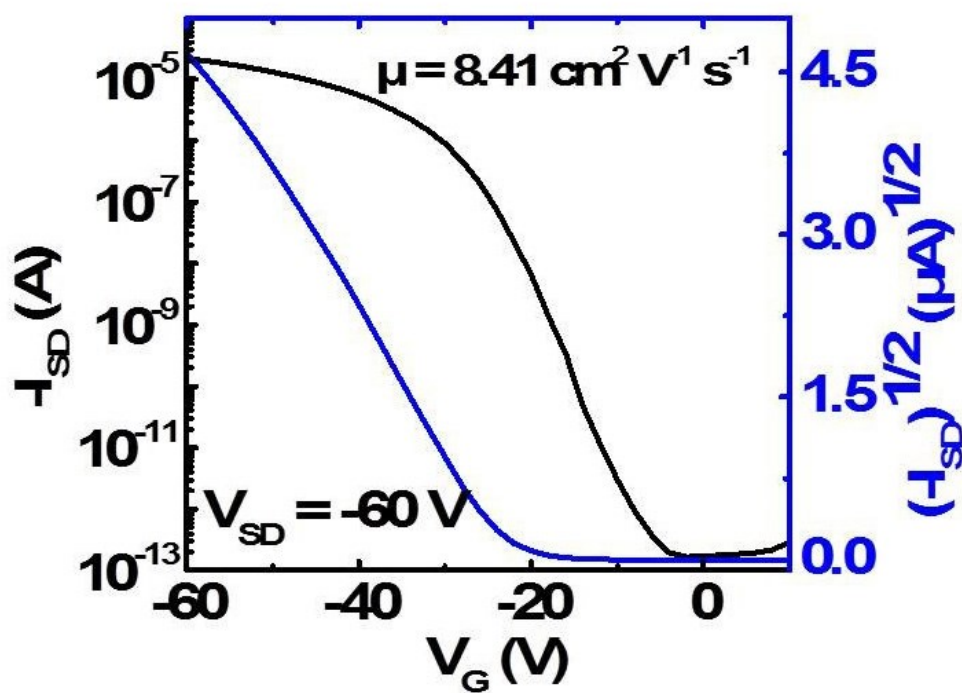


Figure S7. The best OFET based on 1,5-DAN single-crystal with mobility up to 8.41  $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ .

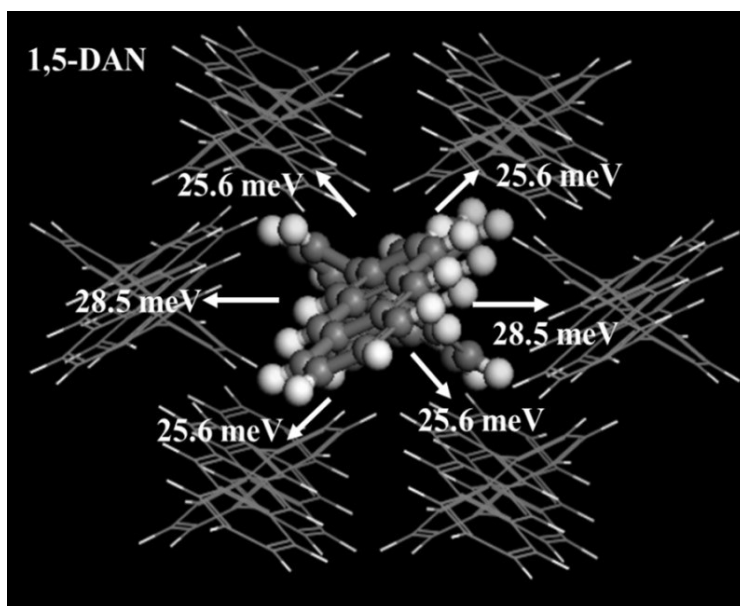


Figure S8. Theoretical calculation of transfer integral of 1,5-DAN single crystal.

Table S2. Summary of high mobility emissive organic semiconductor materials in recent years.

Material	$\mu$ [cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> ]	PLQY [%]	Luminous color	Ref.
2,5-DATT	0.92	46.08	Yellow-green	16
2,6-DAN	19	37.09	Green	24
BDPV2T	1	30	Green	31
Ant-Th-Ph	1.1	36.52	Green	13
Ant-ThPh	4.7	33.32	Blue-green	13
dNaAnt	12.3	29.2	Blue-green	15
DPA	34	41.2	Blue	26
HPVAnt	2.62	70	Blue	32
LD-1	0.25	60.3	Blue	12
DPVA	0.16	42	Green	33
P3V2	0.12	85	Blue	34
P4V3	0.12	52	Green	34
CH3-P3V2	0.17	89	Blue	34
$\beta$ -phase DABD	0.25	20	Orange	35
DPPa	1.6	37.13	Blue	36
DSPa	0.4	62.36	Blue	36
BP3T	1.64	80	Orange	37
AC5	0.29	35	Green	38
1,6-DTEP	2.1	32	Orange	39
2,7-DTEP	0.025	35	Blue-green	39
1,5-DAN	8.41	20.54	Blue	This work