# Supporting Information

## Shifting shades: A polymorph-driven luminescence modulation in a dual-state emissive organic luminophore

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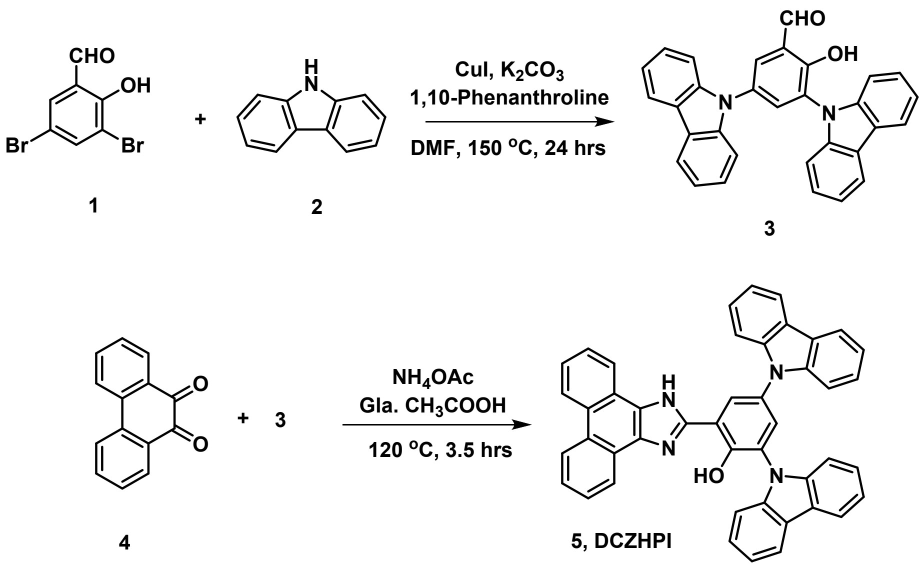
**Table of Contents**

**1. Reaction Scheme for DCZHPI Synthesis**




**Scheme S1**. Synthesis of DCZHPI

**2. General Procedure for the Synthesis of 3,5-Dicarbazole Salicylaldehyde (3)**

A mixture of 3,5-dibromosalicylaldehye **1** (500 mg, 1.786 mmol, 1 equiv.), carbazole **2** (746.5 mg, 4.46 mmol, 2.5 equiv.), 1,10-phenanthroline (96.4 mg, 0.5 mmol, 0.3 equiv.), potassium carbonate (987 mg, 7.14 mmol, 4 equiv.), and CuI (340 mg, 1.785 mmol, 1 equiv.) were taken in round round-bottom flask containing anhydrous DMF under an argon atmosphere. The reaction mixture was heated at 150 °C for 24 hours. After completion of the reaction, the mixture was cooled, quenched with water, and extracted with DCM (3 x 20 mL). The collected organic phases were dried over $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with 3% EtOAc in hexane as the eluent. A pale-yellow powder of compound **3a** was obtained in 40% yield.

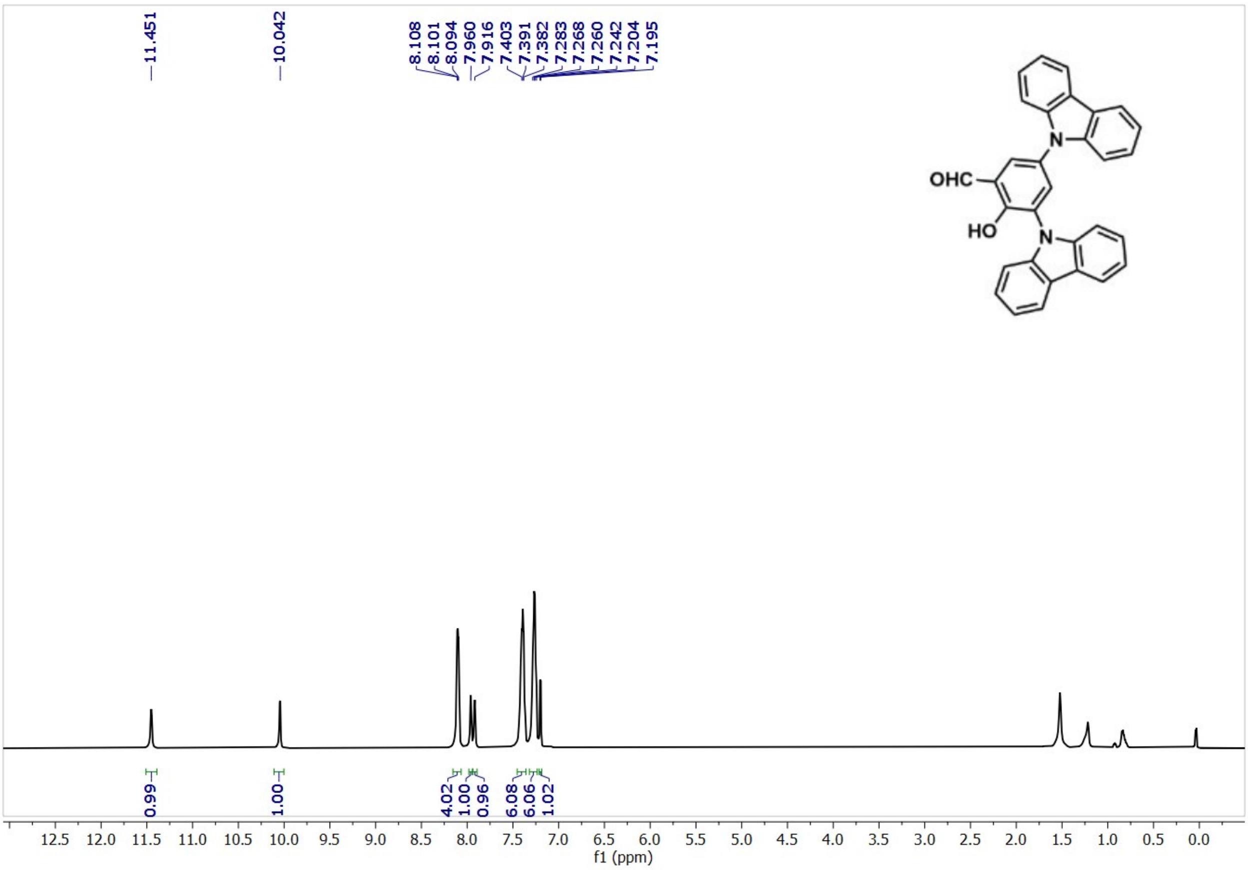
### 3. General Procedure for the synthesis of 3,5-dicarbazole-o-hydroxyphenyl-phenanthroimidazole (5, DCZHPI)

The mixture of **3a** (250 mg, 0.587 mmol, 1 equiv.) and 9,10-phenanthrenedione **4** (122 mg, 0.587 mmol, 1 equiv.) and ammonium acetate (452 mg, 5.87 mmol, 10 equiv.) was dissolved in glacial acetic acid under an argon atmosphere. The reaction mixture was refluxed for 3.5 hours in a magnetic stirrer. After completion of the reaction, the solid residue was filtered and further purified using column chromatography on silica gel with 7% EtOAc in hexane as the eluent. Compound **DCZHPI** was obtained as a white powder (55% yield).

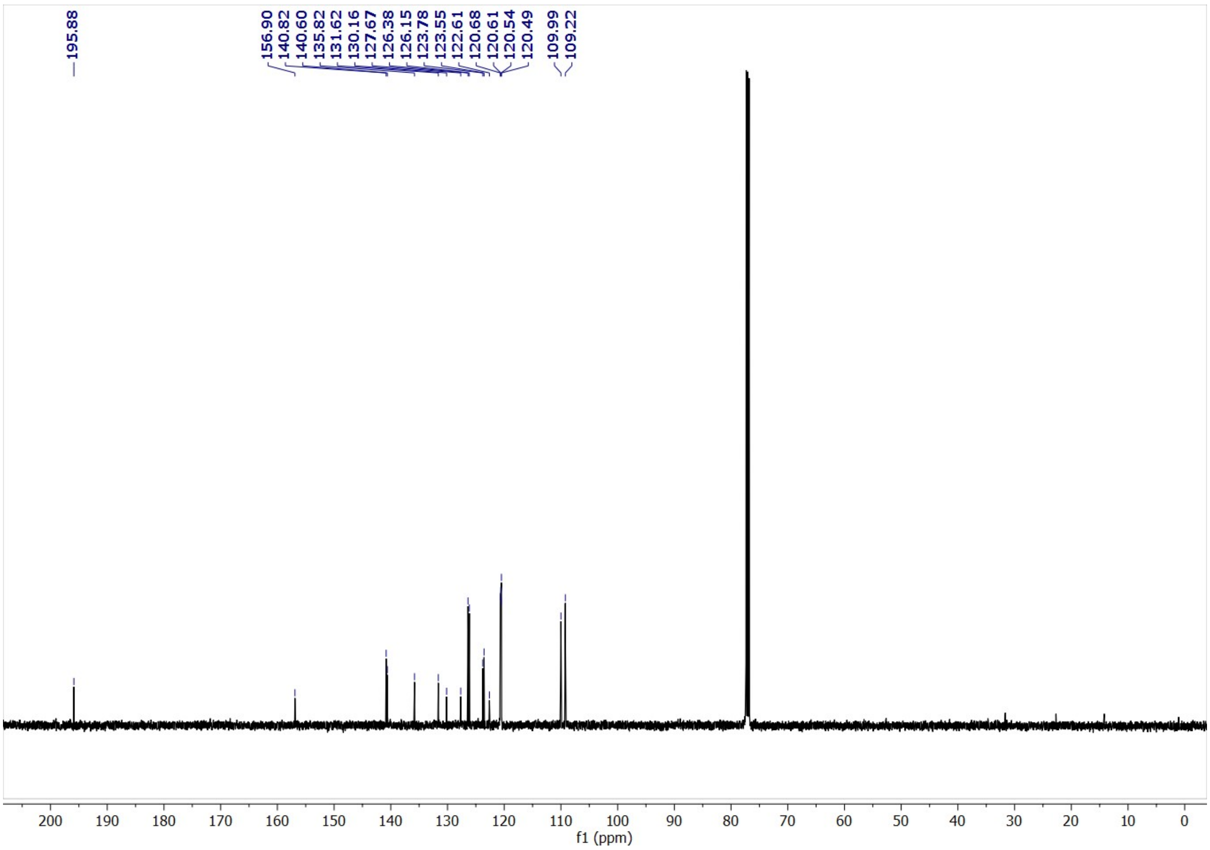
### 4. Characterization Data for 3,5-Dicarbazole Salicylaldehyde (3)

Yellow solid (yield: 300 mg, 40%). $^{1}$H NMR (500 MHz, $CDCl_3$): $\delta$ 11.45 (s, 1H), 10.04 (s, 1H), 8.10-8.09 (m, 4H), 7.96 (s, 1H), 7.91 (s, 1H), 7.40- 7.38 (m, 6H), 7.28-7.24 (m, 6H), 7.20-7.19 (s, $J$=5 Hz, 1H). $^{13}$C {$^{1}$H} NMR (126 MHz, $CDCl_3$): $\delta$ 195.8, 156.9, 140.8, 140.6, 135.8, 131.6, 130.1, 127.6, 126.3, 126.1, 123.7, 123.5, 122.6, 120.7, 120.6, 120.5,120.4, 109.9, 109.2 .

### 5. Figure S1: $^{1}$H NMR of 3,5-Dicarbazole Salicylaldehyde (3)



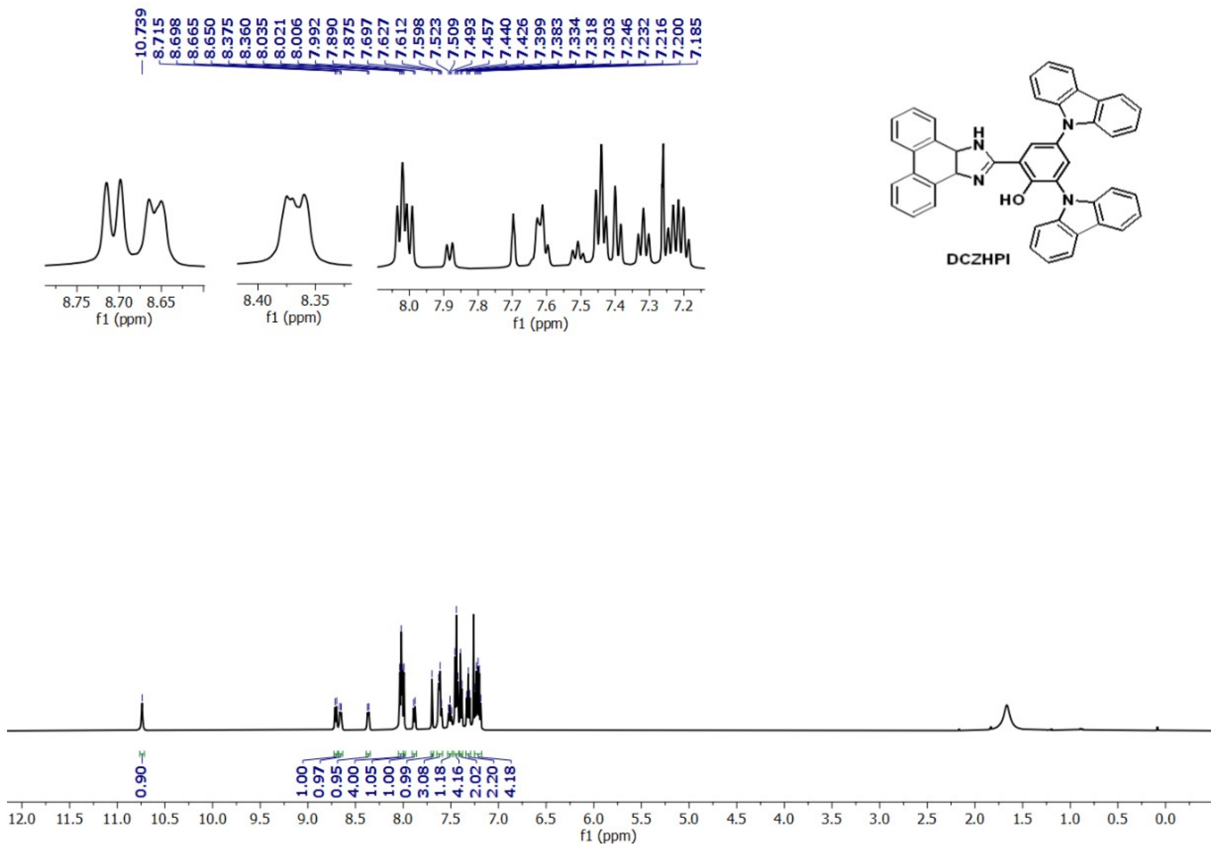
## 6. Figure S2: $^{13}$C NMR of 3,5-Dicarbazole Salicylaldehyde (3)



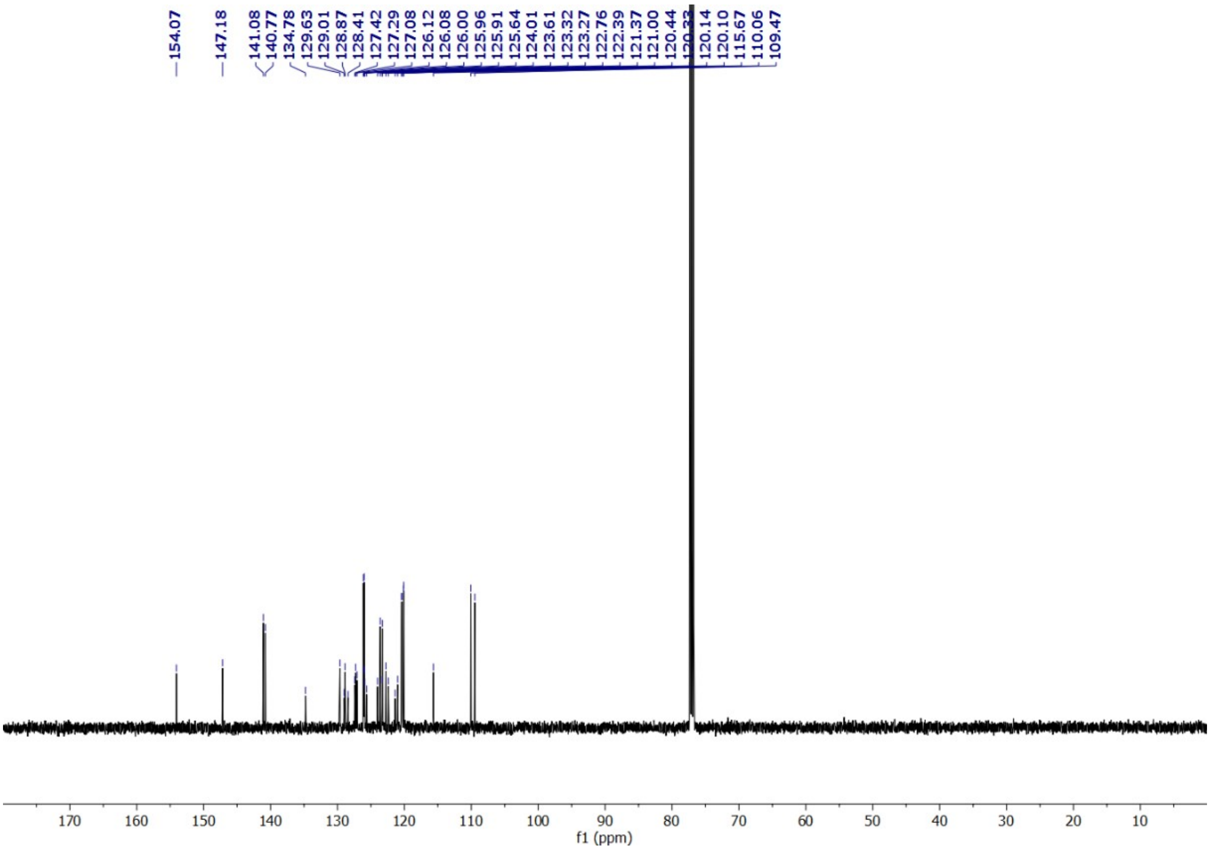

## 7. Characterization Data for DCZHPI (5)

White solid (yield: 206 mg, 55%). $^1$H NMR (500 MHz, $CDCl_3$): $\delta$ 10.74 (s,1H), 8.71-8.69 (d, $J$ = 8.5 Hz, 1H), 8.66-8.65 (d, $J$ = 7.5Hz, 1H), 8.37-8.36 (d, $J$ = 7.5Hz, 1H), 8.03-8.01 (t, $J$ = 14.5 Hz,4H), 7.99 (s, 1H), 7.89-7.87 (d, $J$ = 7.5 Hz, 1H), 7.69 (s, 1H), 7.63-7.59 (m, 3H), 7.52-7.49 (t, $J$ = 7 Hz, 1H), 7.46-7.43 (t, $J$ = 8.5 Hz, 4H), 7.39-7.38 (d, $J$=8 Hz 2H), 7.33-7.30 (t, $J$ = 8 Hz, 2H), 7.25-7.18 (m, 4H). $^{13}$C {$^1$H} NMR (126 MHz, $CDCl_3$): $\delta$ 154.0, 147.1, 141.0, 140.7, 134.7, 129.6, 129.0, 128.8, 128.4, 127.4, 127.2, 127.0, 126.1, 126.0, 126.0, 125.9, 125.9, 125.6, 124.0, 123.6, 123.3, 123.2, 122.7, 122.3, 121.3, 121.0, 120.4, 120.3, 120.1, 120.1, 115.6, 110.0, 109.4. HRMS (ESI, $m/z$): calcd for $C_{45}H_{28}N_4O$ $(M+H)^+$: 641.2336, found: 641.2346.

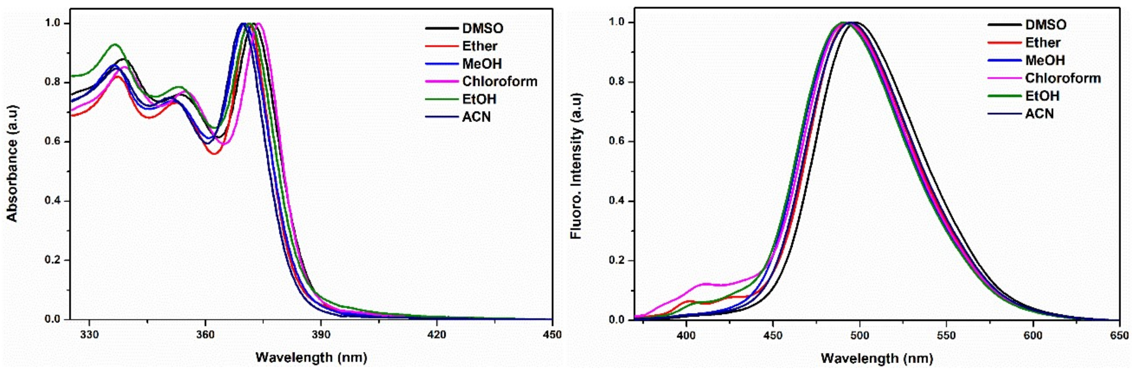
## 8. Figure S3: $^{1}$H NMR of DCZHPI



## 9. Figure S4: $^{13}$C NMR of DCZHPI




## 10. Figure S5: UV Vis absorption and PL emission spectra of DCZHPI in various solvents




## 11. Table S1: Photophysical parameters of DCZHPI in various solvents

| | $\lambda_{abs}$ (nm) | $\lambda_{em}$ (nm) | Stokes shift (nm) | $\Phi_F$ | $<\tau>_F$ (ns) | $K_r$ (ns)$^{-1}$ | $K_{nr}$ (ns)$^{-1}$ |
|---|---|---|---|---|---|---|---|
| **Ether** | 371 | 493 | 122 | 0.52 | 4.58 | 0.1135 | 0.1048 |
| **CHCl3** | 370 | 490 | 120 | 0.57 | 4.55 | 0.1252 | 0.0945 |
| **EtOH** | 371 | 491 | 120 | 0.55 | 4.90 | 0.1122 | 0.0918 |
| **MeOH** | 369 | 492 | 123 | 0.56 | 4.95 | 0.1131 | 0.0889 |
| **ACN** | 369 | 494 | 125 | 0.51 | 4.83 | 0.1055 | 0.1015 |
| **DMSO** | 372 | 497 | 125 | 0.53 | 4.95 | 0.1070 | 0.0950 |

Note: Radiative and non-radiative rates ($k_r$, $k_{nr}$) were calculated using equations $k_r = \phi_F / \tau_F$ and $\tau_F = (k_r + k_{nr})^{-1}$, respectively.

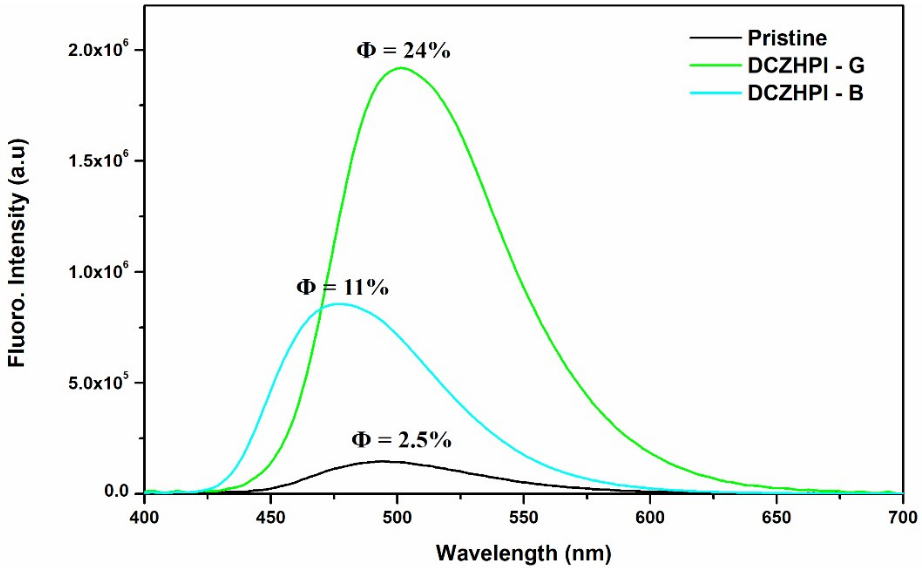
**12. Table S2: Time-resolved PL parameters of DCZHPI polymorphs**

| | $\lambda_{em}$ (nm) | $\tau_1$ (ns) | $\tau_2$ (ns) | $a_1$ | $a_2$ | $f_1$ (%) | $f_2$ (%) | $<\tau>$ (ns) | $\chi^2$ |
|---|---|---|---|---|---|---|---|---|---|
| **Pristine** | 495 | 0.2 | 2.5 | 59.95 | 40.05 | 10.69 | 89.31 | 2.25 | 1.24 |
| **DCZHPI B** | 478 | 0.14 | 2.39 | 31.42 | 68.58 | 2.61 | 97.39 | 2.33 | 1.03 |
| **DCZHPI G** | 503 | 0.02 | 3.5 | 56.12 | 43.88 | 0.73 | 99.27 | 3.48 | 1.27 |

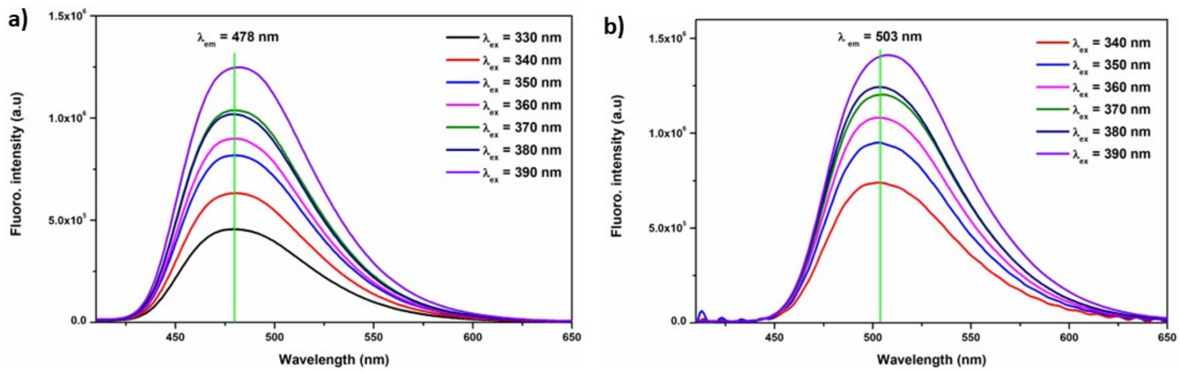
**13. Table S3: Photophysical parameters of DCZHPI in different polymorphs**

| | $\lambda_{em}$ (nm) | Stokes shift (nm) | $<\tau>_F$ (ns) | $K_r$ (ns)$^{-1}$ | $K_{nr}$ (ns)$^{-1}$ |
|---|---|---|---|---|---|
| **Pristine** | 495 | 125 | 2.25 | 0.011 | 0.433 |
| **DCZHPI B** | 478 | 108 | 2.33 | 0.047 | 0.382 |
| **DCZHPI G** | 503 | 133 | 3.48 | 0.069 | 0.218 |

**14. Figure S6: PL emission spectra of DCZHPI in different polymorphs**



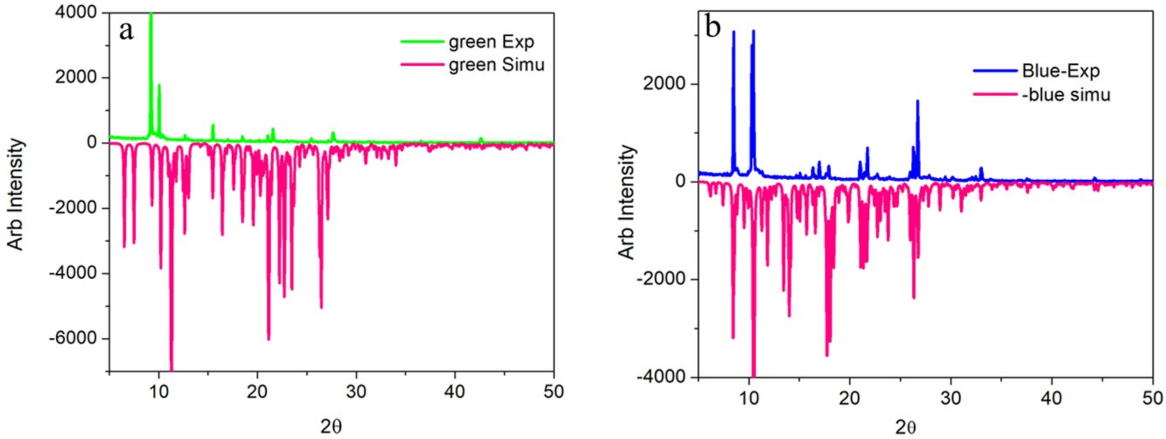

**15. Figure S7: PL emission spectra at different excitation wavelengths of polymorph (a) DCZHPI B and (b) DCZHPI G.**



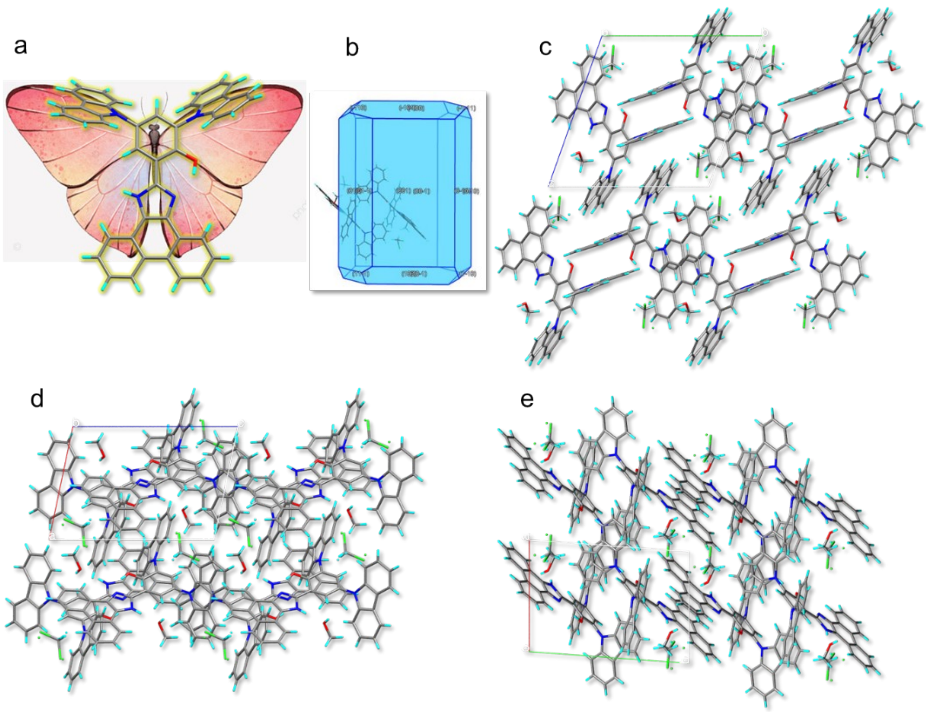

## 16. Crystallographic studies

Single-crystal X-ray Diffraction: Data for **DCZHPI-G** and **DCZHPI-B** were collected at 298 K on a Bruker D8 Quest diffractometer that used MoKα radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.38A (included APEX 5 software suite, v 2017.3-0) and a multi-scan absorption correction using SADABS unknown version was applied[1-3]. The structure was solved by dual methods with SHELXT and refined by full-matrix least-squares methods against F2 using SHELXL 2019/3, all included in APEX 5 software[4,5]. All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their Uiso values constrained to 1.5 times the Ueq of their pivot atoms for terminal sp3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond length restraints and displacement parameter restraints. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre[6]. CCDC 2480006 and 2414467 contain the supplementary crystallographic data for this paper. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

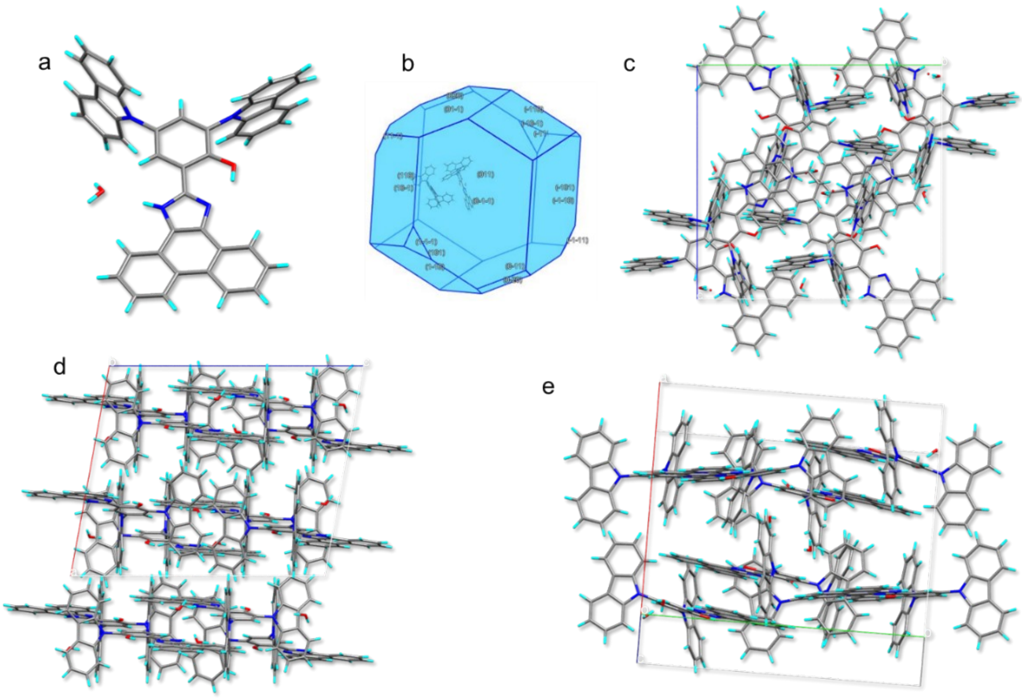
**17. Figure S8. Experimental and simulated PXRD patterns of (a) DCZHPI-G and (b) DCZHPI-B.**



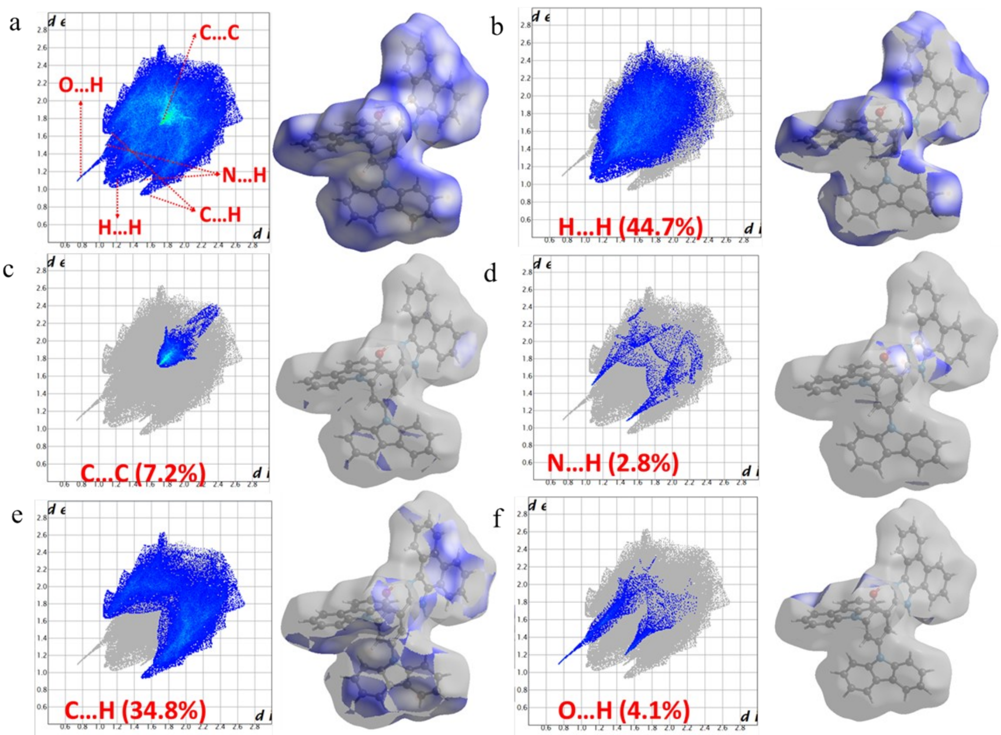

**18. Figure S9. Packing diagram of the DCZHPI-G crystal. (a) molecular conformation and (b) BFDH morphology, (c, d, e) packing structures viewed from different axes.**



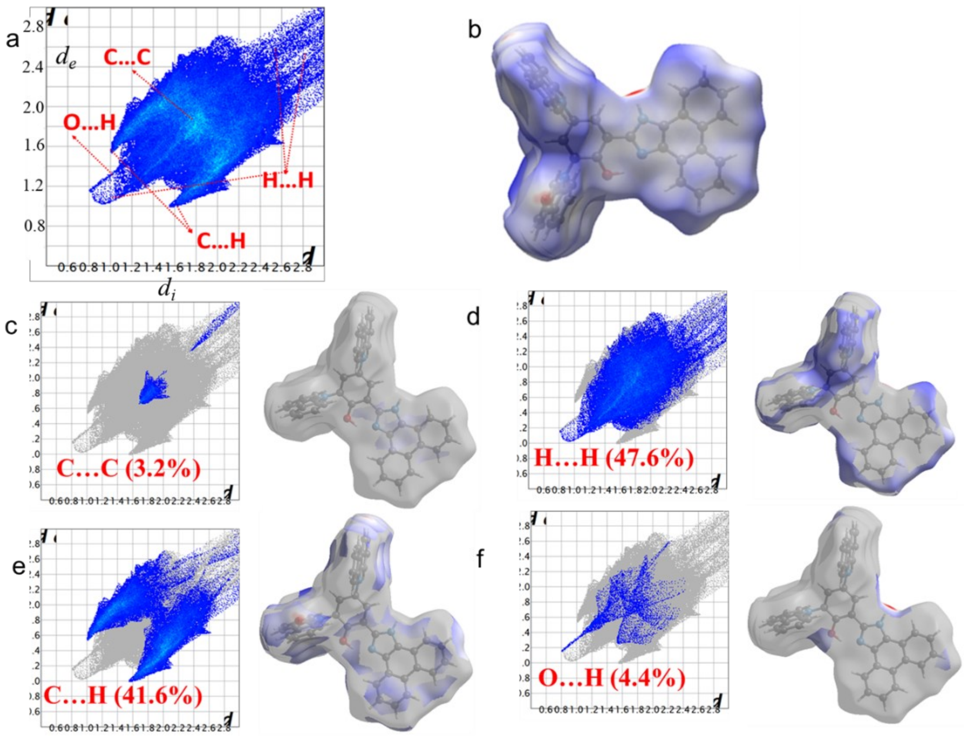
**19. Figure S10. (a) Packing diagram of the DCZHPI-B crystal. (a) molecular conformation and (b) BFDH morphology, (c, d, e) packing structures viewed from different axes**




**20. Figure S11. Hirshfeld Surface analysis of DCZHPI-G crystal showing contribution of various intermolecular interactions (lattice solvent molecules were omitted during calculation due to having disorder).**



**21. Figure S12. Hirshfeld Surface analysis of DCZHPI-B crystal showing contribution of various intermolecular interactions (lattice solvent molecules were omitted during calculation due to having disorder).**




**22. Table S4. Crystallographic parameters of DCZHPI-G and DCZHPI-B.**

| | **DCZHPI-G** | **DCZHPI-B** |
|---|---|---|
| CCDC number | 2480006 | 2414467 |
| Empirical formula | $C_{47}H_{34}Cl_2N_4O_2$ | $C_{90}H_{62}N_8O_5$ |
| Formula weight | 757.68 | 1335.47 |
| Temperature [K] | 298 | 298 |
| Crystal system | triclinic | monoclinic |
| Space group (number) | $P1$ (2) | $P2_1/n$ (14) |
| $a$ [Å] | 9.6774(7) | 17.13531(10) |
| $b$ [Å] | 14.4259(9) | 20.91655(11) |
| $c$ [Å] | 14.6505(9) | 20.35341(14) |
| α [°] | 109.181(2) | 90 |
| β [°] | 101.131(2) | 100.4016(6) |
| γ [°] | 90.266(2) | 90 |
| Volume [Å$^3$] | 1890.3(2) | 7175.02(8) |
| $Z$ | 2 | 4 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.331 | 1.236 |
| $\mu$ [mm$^{-1}$] | 0.218 | 0.615 |
| $F$(000) | 788 | 2792 |

| | | |
|---|---|---|
| Crystal size [$mm^3$] | 0.14×0.15×0.2 | 0.15×0.15×0.2 |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) | Cu $K_\alpha$ (λ=1.54184 Å) |
| 2θ range [°] | 4.30 to 52.04 (0.81 Å) | 6.22 to 136.22 (0.83 Å) |
| Index ranges | −11 ≤ h ≤ 11−17 ≤ k ≤ 17−18 ≤ l ≤ 18 | −20 ≤ h ≤ 20−25 ≤ k ≤ 25−20 ≤ l ≤ 24 |
| Reflections collected | 21040 | 112520 |
| Independent reflections | 6912 $R_{int}$ = 0.1691 $R_{sigma}$ = 0.1109 | 13054 $R_{int}$ = 0.0329 $R_{sigma}$ = 0.0172 |
| Completeness to θ = 25.242° | 92.9 % | 99.8 % |
| Data / Restraints / Parameters | 6912 / 470 / 519 | 13054 / 1 / 940 |
| Absorption correction $T_{min}/T_{max}$ (method) | 0.5111 / 0.7453 (multi-scan) | 0.6411 / 1.0000 (multi-scan) |
| Goodness-of-fit on $F^2$ | 1.197 | 1.026 |
| Final $R$ indexes [$I≥2σ(I)$] | $R_1$ = 0.1164 w$R_2$ = 0.2849 | $R_1$ = 0.0479 w$R_2$ = 0.1434 |
| Final $R$ indexes [all data] | $R_1$ = 0.1559 w$R_2$ = 0.3547 | $R_1$ = 0.0576 w$R_2$ = 0.1528 |
| Largest peak/hole [$eÅ^{-3}$] | 0.64/−0.46 | 0.56/−0.20 |
| Extinction coefficient | 0.15(2) | 0.00028(4) |

**23. Table S5. Hydrogen bonding in the DCZHPI-G crystal**

| **D–H···A [Å]** | **d(D–H) [Å]** | **d(H···A) [Å]** | **d(D···A)[Å]** | **<(DHA)[°]** |
|---|---|---|---|---|
| O2–H2···N3 | 0.82 | 1.87 | 2.608(3) | 148.4 |
| C6–H6···O4 | 0.93 | 2.54 | 3.454(4) | 166.0 |

**24. Table S6. Hydrogen bonding in the DCZHPI-B crystal**

| **D–H···A [Å]** | **d(D–H) [Å]** | **d(H···A) [Å]** | **d(D···A) [Å]** | **<(DHA) [°]** |
|---|---|---|---|---|
| O1–H1···N2 | 0.82 | 1.83 | 2.5639(18) | 147.9 |
| O3–H3A···O5 | 0.85 | 2.09 | 2.867(7) | 151.3 |

## 25. Quantum Yield Calculations

The quantum yield was determined with reference to quinine sulfate (QS) in 0.1 M $H_2SO_4$ using the following formula[7,8] .

$$\Phi_{sample} = \Phi_{ref} * (OD_{ref} / OD_{sample})*( I_{ref} / I_{sample})* (\mu^2_{solvent} /\mu^2_{ref})$$

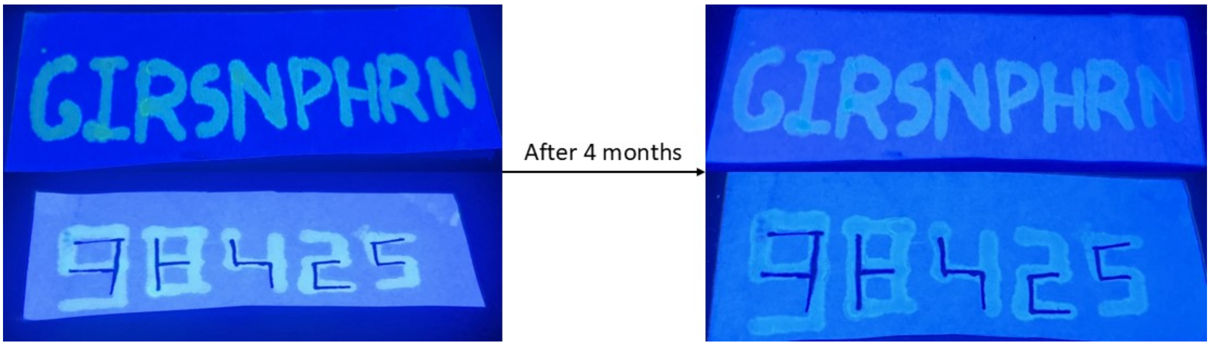
Where, $\Phi_{sample}$ = quantum yield of sample; $\Phi_{ref}$ = quantum yield of reference; $I_{sample}$ = area under PL curve of sample; $I_{ref}$ = area under PL curve of reference; $OD_{ref}$ = absorbance of the reference; $OD_{sample}$ = absorbance of the sample; $\mu^2_{solvent}$ = refractive index of solvent ; $\mu^2_{ref}$ = refractive index of reference.

**$\Phi_{sample}$= 0.57 in Chloroform (ref. $\Phi_{ref}$= 0.54)**

## 26. Data Encryption for Anticounterfeit Studies

For data encryption, $10^{-7}$ M concentrated solution of **DCZHPI** in DCM was used. The letters were written on Whatman filter papers using TLC capillaries. The data encrypted papers were kept in the ambient atmosphere over a long period to check the stability, and depicted in **Figure S13**. Importantly, the UV on/off cycling experiments using data-encrypted paper confirm the photostability of the material.

**Figure S13: Data encryption using DCZHPI**




## 27. Theoretical Calculations and Tables S7, S8, S9, S10 and Figures S14, S15

Density functional theory (DFT) and time-dependent DFT (TD-DFT)[9], with Gaussian 16 package[10] and B3LYP/6-31G+(d,p) level[11,12] was employed.

**TABLE S7:** Energy difference of between optimized geometry (single molecule, gas phase, B3lyp/6-31+g(d,p)) of enol-form and keto-form of DCZHPI.

| **Tautomer (E in Hartree)** | **Energy difference** | | |
|---|---|---|---|
| | Hartree (au) | kcal/mol | eV |
| Enol (-2026.005853) | 0.00603 | 3.784 | 0.16408 |
| Keto (-2025.999823) | | | |

**Figure S14.** Geometry optimized (single molecule, gas phase, B3lyp/6-31+g(d,p)) structures of enol-form and keto-form

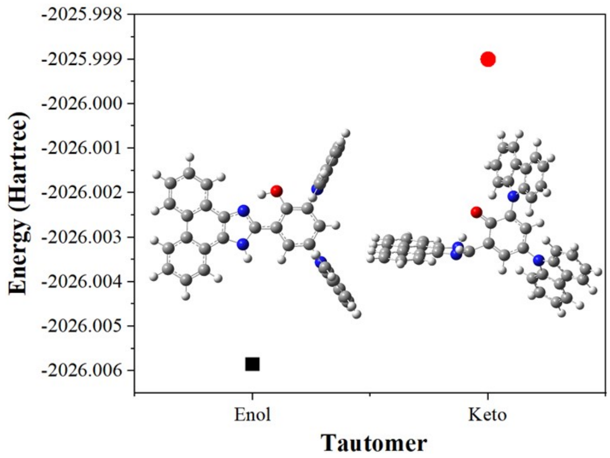



**Figure S15**. TDDFT (B3lyp/6-31+g(d,p), gas phase single molecule) calculated spectra of **enol-form** showing orbital contribution and oscillator strength (OS).

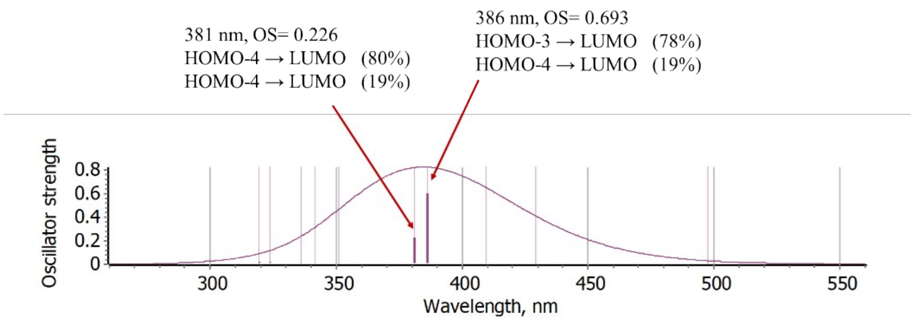



**Table S8.** Calculated electronic transitions and related FMO contribution

| **Compound** | **Calculated $\lambda_{max}$** | **Oscillator strength (*f*)** | **MO transition (% contribution)** |
|---|---|---|---|
| DCZHPI (Enol) | 386.5 nm | 0.693 | HOMO-4-LUMO (19 %)<br>HOMO-3-LUMO (78 %) |

| | | | |
|---|---|---|---|
| | 381 nm | 0.226 | HOMO-4-LUMO (80 %)<br>HOMO-3-LUMO (19 %) |
| DCZHPI (keto) | 569.8 nm | 0.034 | HOMO-5-LUMO (73 %)<br>HOMO-4-LUMO (17 %)<br>HOMO-2-LUMO (7 %) |
| | 612 nm | 0.005 | HOMO-2-LUMO (93 %)<br>HOMO-5-LUMO (6 %) |

**Table S9**. Geometry optimized (B3lyp/6-31+g(d,p, gas phase single molecule) coordinates of the enol form

| | | | |
|---|---|---|---|
| 6 | -6.357138000 | 3.229255000 | -0.018103000 |
| 6 | -5.161326000 | 2.533103000 | -0.017157000 |
| 6 | -5.144793000 | 1.121349000 | -0.007497000 |
| 6 | -6.371515000 | 0.384929000 | 0.001375000 |
| 6 | -7.573761000 | 1.133786000 | 0.000087000 |
| 6 | -7.573119000 | 2.519435000 | -0.009358000 |
| 6 | -3.911755000 | 0.382569000 | -0.005566000 |
| 6 | -6.358734000 | -1.081121000 | 0.011062000 |
| 6 | -5.107690000 | -1.790118000 | 0.010834000 |
| 6 | -3.923061000 | -1.009737000 | 0.003203000 |
| 6 | -5.102895000 | -3.208894000 | 0.018634000 |
| 1 | -4.154922000 | -3.740964000 | 0.016718000 |
| 6 | -6.285318000 | -3.924826000 | 0.027441000 |
| 6 | -7.517115000 | -3.241379000 | 0.028610000 |
| 6 | -7.540983000 | -1.853471000 | 0.020363000 |
| 1 | -6.358573000 | 4.315560000 | -0.025646000 |

| | | | |
|---|---|---|---|
| 1 | -4.212230000 | 3.059572000 | -0.023960000 |
| 1 | -8.528801000 | 0.620817000 | 0.006485000 |
| 1 | -8.517210000 | 3.056943000 | -0.010112000 |
| 1 | -6.263430000 | -5.010926000 | 0.033153000 |
| 1 | -8.449532000 | -3.797728000 | 0.035603000 |
| 1 | -8.505608000 | -1.358476000 | 0.021094000 |
| 6 | -1.813702000 | -0.231971000 | -0.004880000 |
| 6 | -0.399855000 | -0.174623000 | -0.004389000 |
| 6 | 0.239951000 | 1.118039000 | -0.004715000 |
| 6 | 0.456036000 | -1.328700000 | -0.002311000 |
| 6 | 1.623114000 | 1.190752000 | -0.001770000 |
| 6 | 1.843734000 | -1.205955000 | 0.000497000 |
| 1 | 0.032329000 | -2.327479000 | -0.004709000 |
| 6 | 2.472083000 | 0.042254000 | 0.001117000 |
| 1 | 3.550436000 | 0.133013000 | 0.002053000 |
| 8 | -0.479613000 | 2.259087000 | -0.007341000 |
| 1 | -1.462181000 | 1.995371000 | -0.010069000 |
| 6 | 3.157282000 | -3.029760000 | 1.130455000 |
| 6 | 3.130721000 | -3.048967000 | -1.128675000 |
| 6 | 2.950316000 | -2.726685000 | 2.480407000 |
| 6 | 3.965828000 | -4.126138000 | 0.725145000 |
| 6 | 2.892870000 | -2.768134000 | -2.478351000 |
| 6 | 3.948773000 | -4.138456000 | -0.723910000 |
| 6 | 3.569392000 | -3.539972000 | 3.429126000 |

| | | | |
|---|---|---|---|
| 1 | 2.322200000 | -1.891772000 | 2.772935000 |
| 6 | 4.575740000 | -4.927406000 | 1.699502000 |
| 6 | 3.490199000 | -3.597161000 | -3.427387000 |
| 1 | 2.257847000 | -1.938231000 | -2.770248000 |
| 6 | 4.536261000 | -4.955947000 | -1.698577000 |
| 6 | 4.375470000 | -4.629899000 | 3.046949000 |
| 1 | 3.422669000 | -3.329956000 | 4.484891000 |
| 1 | 5.195991000 | -5.771228000 | 1.409727000 |
| 6 | 4.304936000 | -4.680847000 | -3.045804000 |
| 1 | 3.319255000 | -3.404600000 | -4.482830000 |
| 1 | 5.163295000 | -5.794865000 | -1.409157000 |
| 1 | 4.841822000 | -5.244920000 | 3.810783000 |
| 1 | 4.753632000 | -5.308606000 | -3.809850000 |
| 6 | 2.552249000 | 3.237504000 | 1.119809000 |
| 6 | 2.561376000 | 3.231902000 | -1.125220000 |
| 6 | 2.370973000 | 2.879843000 | 2.463734000 |
| 6 | 3.126697000 | 4.481414000 | 0.727764000 |
| 6 | 2.391342000 | 2.867354000 | -2.468817000 |
| 6 | 3.132646000 | 4.477793000 | -0.734692000 |
| 6 | 2.781681000 | 3.798701000 | 3.429314000 |
| 1 | 1.923505000 | 1.928930000 | 2.724331000 |
| 6 | 3.527030000 | 5.378621000 | 1.702195000 |
| 6 | 2.809922000 | 3.781395000 | -3.435576000 |
| 1 | 1.946423000 | 1.914935000 | -2.728293000 |

| | | | |
|---|---|---|---|
| 6 | 3.540966000 | 5.370077000 | -1.710300000 |
| 6 | 3.350332000 | 5.025827000 | 3.058995000 |
| 1 | 2.656553000 | 3.562016000 | 4.480090000 |
| 1 | 3.965660000 | 6.336838000 | 1.442628000 |
| 6 | 3.375393000 | 5.010444000 | -3.066736000 |
| 1 | 2.693603000 | 3.539359000 | -4.486144000 |
| 1 | 3.977499000 | 6.329588000 | -1.451983000 |
| 1 | 3.660010000 | 5.723694000 | 3.829925000 |
| 1 | 3.691407000 | 5.704444000 | -3.838586000 |
| 7 | 2.656228000 | -2.387736000 | 0.001126000 |
| 7 | 2.228688000 | 2.506252000 | -0.002270000 |
| 7 | -2.629821000 | 0.857970000 | -0.011038000 |
| 7 | -2.585923000 | -1.390674000 | -0.001217000 |
| 1 | -2.232259000 | -2.331777000 | 0.032728000 |

**Table S10**. Geometry optimized (B3lyp/6-31+g(d,p, gas phase single molecule) coordinates of the Keto form

| | | | |
|---|---|---|---|
| 6 | -6.591035000 | -0.452142000 | -3.043359000 |
| 6 | -5.350006000 | -0.625039000 | -2.458016000 |
| 6 | -5.214862000 | -0.679746000 | -1.051218000 |
| 6 | -6.369895000 | -0.570944000 | -0.212071000 |
| 6 | -7.619701000 | -0.394940000 | -0.850545000 |
| 6 | -7.733867000 | -0.332856000 | -2.230396000 |
| 6 | -3.946953000 | -0.825010000 | -0.410888000 |
| 6 | -6.231599000 | -0.652585000 | 1.243246000 |

| | | | |
|---|---|---|---|
| 6 | -4.941202000 | -0.841864000 | 1.833841000 |
| 6 | -3.817194000 | -0.902011000 | 0.954357000 |
| 6 | -4.809396000 | -0.944103000 | 3.238080000 |
| 1 | -3.827145000 | -1.112145000 | 3.670207000 |
| 6 | -5.916621000 | -0.849665000 | 4.061407000 |
| 6 | -7.190210000 | -0.653292000 | 3.495324000 |
| 6 | -7.337543000 | -0.561036000 | 2.120404000 |
| 1 | -6.683707000 | -0.413697000 | -4.124630000 |
| 1 | -4.467843000 | -0.735112000 | -3.082078000 |
| 1 | -8.521181000 | -0.305300000 | -0.255590000 |
| 1 | -8.711139000 | -0.196829000 | -2.683682000 |
| 1 | -5.804255000 | -0.931395000 | 5.138360000 |
| 1 | -8.063627000 | -0.578135000 | 4.136060000 |
| 1 | -8.333577000 | -0.415296000 | 1.718747000 |
| 6 | -1.742917000 | -1.124000000 | 0.053216000 |
| 6 | -0.329966000 | -0.653835000 | -0.045106000 |
| 6 | -0.055993000 | 0.778247000 | -0.059935000 |
| 6 | 0.697083000 | -1.562293000 | -0.054962000 |
| 6 | 1.355550000 | 1.185584000 | -0.109374000 |
| 6 | 2.060320000 | -1.140009000 | -0.078770000 |
| 1 | 0.470655000 | -2.621955000 | -0.001935000 |
| 6 | 2.366013000 | 0.231471000 | -0.089552000 |
| 1 | 3.400787000 | 0.548256000 | -0.159470000 |
| 8 | -0.990221000 | 1.611325000 | 0.006561000 |

| | | | |
|---|---|---|---|
| 6 | 4.263803000 | -2.103608000 | 0.642658000 |
| 6 | 3.112021000 | -3.226504000 | -0.974368000 |
| 6 | 4.667667000 | -1.232099000 | 1.657905000 |
| 6 | 5.038748000 | -3.236156000 | 0.291102000 |
| 6 | 2.209465000 | -3.614457000 | -1.969566000 |
| 6 | 4.307220000 | -3.948868000 | -0.738970000 |
| 6 | 5.882005000 | -1.491624000 | 2.295129000 |
| 1 | 4.062611000 | -0.384761000 | 1.954446000 |
| 6 | 6.250727000 | -3.479218000 | 0.945155000 |
| 6 | 2.502079000 | -4.768402000 | -2.698038000 |
| 1 | 1.315455000 | -3.041809000 | -2.184781000 |
| 6 | 4.581592000 | -5.100658000 | -1.483468000 |
| 6 | 6.671636000 | -2.598447000 | 1.941331000 |
| 1 | 6.217584000 | -0.823568000 | 3.082382000 |
| 1 | 6.852034000 | -4.345603000 | 0.685935000 |
| 6 | 3.670173000 | -5.510889000 | -2.456005000 |
| 1 | 1.812358000 | -5.091824000 | -3.471516000 |
| 1 | 5.495636000 | -5.661815000 | -1.313068000 |
| 1 | 7.611835000 | -2.772979000 | 2.454974000 |
| 1 | 3.868896000 | -6.403909000 | -3.040218000 |
| 6 | 2.627834000 | 3.187674000 | 0.668705000 |
| 6 | 1.257764000 | 3.480431000 | -1.126622000 |
| 6 | 3.277773000 | 2.706879000 | 1.809512000 |
| 6 | 2.807132000 | 4.521725000 | 0.225520000 |

| | | | |
|---|---|---|---|
| 6 | 0.372818000 | 3.310797000 | -2.193911000 |
| 6 | 1.942834000 | 4.702821000 | -0.923978000 |
| 6 | 4.141693000 | 3.570901000 | 2.483839000 |
| 1 | 3.103116000 | 1.702543000 | 2.177624000 |
| 6 | 3.676523000 | 5.371594000 | 0.917932000 |
| 6 | 0.167712000 | 4.394207000 | -3.046547000 |
| 1 | -0.160744000 | 2.381122000 | -2.342476000 |
| 6 | 1.719229000 | 5.779902000 | -1.790761000 |
| 6 | 4.348210000 | 4.888814000 | 2.040903000 |
| 1 | 4.655764000 | 3.217962000 | 3.372952000 |
| 1 | 3.818631000 | 6.397579000 | 0.590967000 |
| 6 | 0.828409000 | 5.620605000 | -2.849398000 |
| 1 | -0.525012000 | 4.288298000 | -3.876127000 |
| 1 | 2.238453000 | 6.722416000 | -1.642651000 |
| 1 | 5.026204000 | 5.538175000 | 2.586111000 |
| 1 | 0.642074000 | 6.446309000 | -3.529269000 |
| 7 | 3.082424000 | -2.100827000 | -0.125447000 |
| 7 | 1.683124000 | 2.552072000 | -0.154389000 |
| 7 | -2.682325000 | -0.959873000 | -0.991857000 |
| 7 | -2.469015000 | -1.087559000 | 1.265997000 |
| 1 | -2.064505000 | -0.652235000 | 2.087241000 |
| 1 | -2.437472000 | -0.403702000 | -1.803607000 |