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# **Supporting information**

# Functionalized 1,3-Dipyrrolyl-1,3-diketone Difluoroboron Complexes

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# Table of Contents Materials Characterization......4 Structure of synthesized compounds ......5 Synthesis of compound 1......5 Synthesis of compound 4.....7 Synthesis of compound 5......8 Section 1: NMR spectrum of synthesized compounds ......9 Figure S1: <sup>1</sup>H-NMR spectra of compound 1 in DMSO-d<sub>6</sub>......9 Figure S2: <sup>13</sup>C-NMR spectra of compound 1 in DMSO-d<sub>6</sub>......9 Figure S3: <sup>11</sup>B-NMR spectra of compound 1 in DMSO-d<sub>6</sub>.....10 Figure S4: <sup>19</sup>F-NMR spectra of compound 1 in DMSO-d<sub>6</sub>.....10 Figure S5: <sup>1</sup>H-NMR spectra of compound 2 in DMSO-d<sub>6</sub>......11 Figure S6: <sup>1</sup>H-<sup>1</sup>H COSY Spectra for compound 2 in DMSO-d<sub>6</sub>......11 Figure S7: <sup>13</sup>C-NMR spectra of compound 2 in DMSO-d<sub>6</sub>.....12 Figure S8: <sup>11</sup>B-NMR spectra of compound 2 in DMSO-d<sub>6</sub>.....12 Figure S9: <sup>19</sup>F-NMR spectra of compound 2 in DMSO-d<sub>6</sub>......13 Figure S10: <sup>1</sup>H-NMR spectra of compound 3 in DMSO-d<sub>6</sub>......13 Figure S11: <sup>13</sup>C-NMR spectra of compound 3 in DMSO-d<sub>6</sub>......14 Figure S12: <sup>11</sup>B-NMR spectra of compound 3 in DMSO-d<sub>6</sub>......14 Figure S14: <sup>1</sup>H-NMR spectra of compound 4 in DMSO-d<sub>6</sub>......15 Figure S15: <sup>13</sup>C-NMR spectra of compound 4 in DMSO-d<sub>6</sub>......16

Figure S16: <sup>11</sup> B-NMR spectra of compound 4 in DMSO-d <sub>6</sub> 16
Figure S17: <sup>19</sup> F-NMR spectra of compound 4 in DMSO-d <sub>6</sub> 17
Figure S18: <sup>1</sup> H-NMR spectra of compound 5 in DMSO-d <sub>6</sub> 17
Figure S19: <sup>13</sup> C-NMR spectra of compound 5 in DMSO-d <sub>6</sub> 18
Figure S20: <sup>11</sup> B-NMR spectra of compound 5 in DMSO-d <sub>6</sub> 18
Figure S21: <sup>19</sup> F-NMR spectra of compound 5 in DMSO-d <sub>6</sub> 19
Section 2: Mass spectrometry for synthesized compounds20
Figure S22: MS of compound 120
Figure S23: MS for compound 220
Figure S24: MS for compound 321
Figure S25: MS for compound 421
Figure S26: MS for compound 522
Section 3: Single crystal XRD data23
Table S1: Summary of crystallographic data for 2 and 4
Figure S27: ORTEP plots of (A) compound 2 and (B) compound 4 at 50% probability level24
Table S2: Bond lengths (Å) and bond angles (deg, $^{\circ}$ ) of intermolecularhydrogen bonding interactions in compound 4.24
Section 4: Computational data25
Figure S28: Optimized geometries along with molecular orbitals, HOMO-1, HOMO, LUMO, and LUMO+1 for compounds 1-525
Table S3: Cartesian coordinates of the optimized geometries ofcompounds 1-5 in the isolated state with their total energies representedas E (in eV)
Table S4: HOMO to LUMO orbital contributions from $S_0 \rightarrow S_1$ state along with the corresponding oscillator strengths obtained from TD- B3LYP/6-31G+(d,p) in dichloromethane29
Section 5: Photophysical characterization30
Figure S29: Time-resolved fluorescence decay profiles for compounds (A) 4 (B) 5 in CH <sub>2</sub> Cl <sub>2</sub> solvent30
Figure S30: Time-resolved fluorescence decay profile for compound 2 indifferent solvents
Table S5: TCSPC studies for compound 2 in different solvents

Figure S31: Comparison of the photostabilities of compounds (A) 2, (B) 3,
(C) 4, (D) 5 in acetonitrile (5×10 <sup>-6</sup> M) under continuous UV irradiation
(319 nm) over 3 h
Figure S32: Change of optical density of compounds 2-5 at the absorption maximum wavelength ( $\lambda_{max}$ ) in acetonitrile (5×10 <sup>-6</sup> M) under UV irradiation (319 nm) over 3 h
Figure S33: Normalized absorption spectra of compounds (A) 1, (B) 2, (C) 3, (D) 4 and (E) 5 in various solvents32
Table S6: Experimental photophysical properties of compounds 1-5 invarious solvents
Section 6: Electrochemical studies34
Figure S34: Electrochemical redox data of compounds 1-5 (blue - oxidation, red - reduction) in acetonitrile containing 0.1 M tetrabutylammonium perchlorate as a supporting electrolyte recorded at a scan rate of 100 mV/sec (1 and 2), 50 mV/sec (3, 4 and 5),
References 35
INTEL CHECK

## Materials:

All the solvents and reagents used for synthesizing compounds were obtained commercially with purity >99% or synthesized. The solvents used were anhydrous or analytical grade. Pyrrole and malonyl chloride were purchased from TCI Chemicals (India) Pvt. Ltd. 1,3-Dipyrrol-2'-yl-1,3-propanedione and its BF<sub>2</sub> complex were synthesized as per the literature.<sup>1</sup>

## **Materials Characterization**

<sup>1</sup>H NMR spectra were recorded on a JEOL 500 MHz NMR spectrometer and <sup>13</sup>C NMR spectra were recorded at a 126 MHz magnetic field. <sup>11</sup>B NMR was recorded at 160 MHz and 128 MHz. <sup>19</sup>F NMR were recorded at 471 MHz and 376 MHz. DMSO-d<sub>6</sub> was used as a deuterated solvent to record the NMR spectra. Absorption spectra for solution and solid state were obtained using Analytical Spectro 2080+ and Lambda 950 by Perkin Elmer, Singapore respectively. PL measurements were carried out using Hitachi FL4100 Fluorescence Spectrophotometer equipped with FL solutions software. FT-IR measurements were determined using Thermo Scientific Nicolet Summit X instrument having Everest ATR accessory in solid state. Time-correlated single photon counting (TCSPC) measurements for obtaining the lifetimes and absolute quantum yields were measured on FLS1000, Edinburgh Instruments, UK, and data fitting was carried out using Fluoracle software.

Cyclic Voltammetry measurements were carried out using Gamry instrument potentiostat Interface 1010E-31184 in a three-electrode electrochemical cell with a scan rate of 100 mV/s and 50 mV/s. The measurements used anhydrous acetonitrile as a solvent with tetrabutylammonium perchlorate (TBAP) as a supporting electrolyte. A glassy carbon electrode was used as the working electrode, Ag/AgCl as the reference electrode, and Pt wire as an auxiliary electrode. Ferrocene oxidation was measured for internal calibration before each measurement.

Gaussian 09W program<sup>2</sup> package was used for computational studies. The density functional theory (DFT) hybrid function B3LYP in combination with basis set 6-31G (d, p)<sup>3</sup> was utilized to optimize the structure of all the compounds, except compound containing I (compound-3) where LanL2DZ basis set was employed. The functional hybrid set and identical

basis were used to obtain the oscillator strengths. The oscillator strengths were carefully studied using TD-DFT based on the optimized structures in the  $S_0$  state.

# Structure of synthesized compounds



## **Experimental section**

#### Synthesis of compound 1

 $BF_3 \cdot OEt_2$  (1.53 mL, 12.36 mmol) was added to the solution containing dipyrrolyldiketone<sup>1</sup> (500 mg, 2.47 mmol) in  $CH_2Cl_2$  (90 mL), stirred for 15 minutes at r.t. The crude product was purified with silica gel column chromatography using 1:99 MeOH:  $CH_2Cl_2$ 



as an eluent to afford Compound **1** as an orange solid with 79 % yield. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 12.41 (br, 2H, NH), 7.40-7.35 (m, 2H, pyrrole-H), 7.34-7.29 (m, 2H, pyrrole-H), 7.08 (s, 1H, CH), 6.40-6.36 (m, 2H, pyrrole-H). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 169.42, 129.72, 126.41, 119.75, 113.01, 90.14. <sup>11</sup>B NMR (160 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -0.20. <sup>19</sup>F NMR (471 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -139.16, -139.23. FT-IR ( $\nu$  cm<sup>-1</sup>) = 3449, 3135, 1568, 1529, 1452, 1400, 1337, 1079, 1040, 952, 878, 791, 755, 714. UV/Vis

(CH<sub>2</sub>Cl<sub>2</sub>)  $\lambda_{abs}$  (nm) = 432, Fluorescence (CH<sub>2</sub>Cl<sub>2</sub>) (5µM)  $\lambda_{em}$  (nm) = 451. MS (ESI) m/z: [M+H]<sup>+</sup> calculated for C<sub>11</sub>H<sub>9</sub>BF<sub>2</sub>N<sub>2</sub>O<sub>2</sub> 251.0803, found: 251.0800.

#### Synthesis of compound 2

DMF (6 mL, 78.0 mmol) was taken in a 25 mL round-bottomed flask and cooled to 0  $^{\circ}$ C under an inert atmosphere. POCl<sub>3</sub> (2.8 mL 30.0 mmol) was added dropwise, maintaining 0  $^{\circ}$ C, and stirred for 20 minutes. In another 250 mL two-necked round-bottomed flask, compound **1** (300 mg, 1.20 mmol) was dissolved in 1,2-



dichloroethane and degassed at room temperature. To this solution of compound 1, the aboveprepared reagent was added slowly at room temperature and heated to 55 °C for 2 h. The completion of the reaction was monitored by TLC, and the reaction mixture was quenched using Na<sub>2</sub>CO<sub>3</sub> in ice condition to obtain a neutral pH, followed by stirring for an additional 1 h. The reaction mixture was extracted using dichloromethane/cold water, and the organic layer was concentrated under reduced pressure to obtain the crude product. The crude product was purified with silica gel column chromatography using 20:80 ethyl acetate: pet ether as an eluent, affording compound 2 as a yellow solid with a 30% yield. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>)  $\delta$ (ppm) = 13.19 (br, 1H, NH), 12.77 (br, 1H, NH), 9.74 (s, 1H, CHO), 7.57-7.53 (m, 1H, pyrrole-H), 7.52-7.49 (m, 1H, pyrrole-H), 7.42 (s, 1H, CH), 7.29 (d, J = 4.2 Hz, 1H, pyrrole-H), 7.09 (d, J = 4.2 Hz, 1H, pyrrole-H), 6.50-6.47 (m, 1H, pyrrole-H).<sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 182.31, 171.40, 168.12, 137.93, 132.78, 131.94, 126.46, 122.92, 118.71, 117.72, 114.25, 92.89. <sup>11</sup>B NMR (160 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -0.18. <sup>19</sup>F NMR (376 MHz, DMSO $d_6$ )  $\delta$  (ppm) = -138.85, -138.92. FT-IR ( $\upsilon$  cm<sup>-1</sup>) = 554, 711, 737, 752, 782, 797, 878, 904, 958, 1000, 1031, 1056, 1081, 1131, 1148, 1224, 1264, 1353, 1373, 1412, 1435, 1458, 1486, 1510, 1531, 1568, 1668, 3152, 3259, 3410. UV/Vis (CH<sub>2</sub>Cl<sub>2</sub>)  $\lambda_{abs}$  (nm) = 427, 447. Fluorescence  $(CH_2Cl_2)$  (5µM)  $\lambda_{em}$  (nm) = 467. MS (ESI) m/z = [M+H]<sup>+</sup> calculated for C<sub>12</sub>H<sub>9</sub>BF<sub>2</sub>N<sub>2</sub>O<sub>3</sub> 279.0753, found: 279.0761.

#### Synthesis of compound 3

A 20 mL solution of compound **1** (300 mg, 1.20 mmol) in THF at -5  $^{\circ}$ C to -10  $^{\circ}$ C was treated with N-iodosuccinimide (283.4 mg, 1.26 mmol) in fractions for 20 minutes. The reaction was stirred for an hour at the same temperature and monitored by TLC. After



the formation of mono-iodo product as the major spot on the TLC, the reaction mixture was extracted using ethyl acetate/water. The organic layer was concentrated under reduced pressure using a rotary evaporator to obtain a crude product isolated by silica gel column chromatography using 10:90 ethyl acetate: pet ether to give compound **3** as a yellow solid in 40% yield. Compound **3** exhibited decreased stability in chlorinated solvents over time, resulting in the formation of additional spots. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 12.66 (br, 1H, NH), 12.49 (br, 1H, NH), 7.54-7.52 (m, 1H, pyrrole-H), 7.45-7.41 (m, 2H, pyrrole-H), 7.39-7.36 (m, 1H, pyrrole-H), 7.12 (s, 1H, CH), 6.42-6.38 (m, 1H, pyrrole-H). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 170.09, 167.99, 133.35, 130.64, 128.41, 126.38, 124.94, 120.81, 113.42, 90.69, 65.32. <sup>11</sup>B NMR (160 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -0.23. <sup>19</sup>F NMR (471 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -138.93, -138.99. FT-IR ( $\nu$  cm<sup>-1</sup>) = 591, 616, 665, 716, 754, 786, 816, 840, 879, 902, 913, 961, 1041, 1086, 1227, 1259, 1299, 1327, 1385, 1412, 1452, 1521, 1562, 3130, 3419. UV/Vis (CH<sub>2</sub>Cl<sub>2</sub>)  $\lambda_{abs}$  (nm) = 437, Fluorescence (CH<sub>2</sub>Cl<sub>2</sub>) (5µM)  $\lambda_{em}$  (nm) = 457. MS (ESI) m/z: [M+H]<sup>+</sup> calculated for C<sub>11</sub>H<sub>8</sub>BF<sub>2</sub>IN<sub>2</sub>O<sub>2</sub> 376.9770; found: 376.9767.

#### Synthesis of compound 4

 $HNO_3$  (0.09 mL, 2.38 mmol) was added dropwise to a 50 mL round-bottomed flask containing acetic acid (5.5 mL) at 0 °C. The reaction was stirred for 30 minutes at the same temperature and then added to a 14 mL of cooled acetic acid solution of



compound **1** (350 mg, 1.40 mmol). The reaction was further stirred at 0 °C for 2 h and at room temperature for 1 h and was constantly monitored using TLC. After the completion of the reaction, it was poured into crushed ice and treated with sodium bicarbonate. The reaction mixture was extracted using ethyl acetate/cold water and the organic layer was concentrated at reduced pressure using a rotary evaporator to obtain a crude product. The crude product was purified with silica gel column chromatography using 15:85 ethyl acetate: pet ether as an eluent to obtain compound **4**, which was further recrystallized using CH<sub>2</sub>Cl<sub>2</sub>: Hexane (1:3) to give an orange solid with a 41 % yield. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 14.07 (br, 1H, NH), 12.87 (br, 1H, NH), 7.59-7.52 (m, 2H, pyrrole-H), 7.49 (s, 1H, CH), 7.26 (d, *J* = 4.4 Hz, 1H, pyrrole-H), 7.22 (d, *J* = 4.5 Hz, 1H, pyrrole-H), 6.53-6.49 (m, 1H, pyrrole-H). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 171.21, 166.52, 159.76, 141.39, 133.20, 130.07, 125.97, 116.29, 114.13, 112.02, 92.96. <sup>11</sup>B NMR (160 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -0.22. <sup>19</sup>F NMR (471 MHz,

DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -138.78, -138.84. FT-IR ( $\upsilon$  cm<sup>-1</sup>) = 545, 559, 572, 588, 614, 642, 713, 733, 742, 770, 799, 875, 902, 955, 983, 1023, 1052, 1097, 1251, 1285, 1356, 1393, 1420, 1460, 1511, 1586, 1718, 3145, 3269, 3445. UV/Vis (CH<sub>2</sub>Cl<sub>2</sub>)  $\lambda_{abs}$  (nm) = 436, 452, Fluorescence (CH<sub>2</sub>Cl<sub>2</sub>) (5 $\mu$ M)  $\lambda_{em}$  (nm) = 502. MS (ESI) m/z: [M+NH<sub>4</sub>]<sup>+</sup> calculated for C<sub>11</sub>H<sub>8</sub>BF<sub>2</sub>N<sub>3</sub>O<sub>4</sub> 313.0920; found: 313.0913.

#### Synthesis of compound 5

5% Pd/C (100 mg, 0.93 mmol), was added to a mixture of compound **1** (250 mg, 0.84 mmol), and  $NH_2NH_2 \cdot H_2O$  (0.7 mL) in a solution of 1:1 ratio of MeOH/THF under an inert atmosphere and refluxed for 1 h. After the completion of the reaction, it was



filtered, and the filtrate was concentrated using a rotary evaporator. The crude product was purified with silica gel column chromatography using 25:75 ethyl acetate: pet ether as an eluent to obtain compound **5**, which was further recrystallized using CH<sub>2</sub>Cl<sub>2</sub>: Hexane (1:3) to give a red solid product with 45 % yield. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = 11.69 (br, 1H, NH), 11.19 (br, 1H, NH), 7.41 (d, *J* = 2.2 Hz, 1H, pyrrole-H), 7.00 (d, *J* = 1.5 Hz, 1H, pyrrole-H), 6.91-6.86 (m, 1H, pyrrole-H), 6.57 (s, 1H, CH), 6.49 (s, 2H, NH<sub>2</sub>), 6.20-6.15 (m, 1H, pyrrole-H), 5.69-5.67 (m, 1H, pyrrole-H). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>)  $\delta$  161.13, 153.59, 128.25, 127.45, 124.37, 118.68, 113.38, 110.92, 101.96, 88.01, 55.44. <sup>11</sup>B NMR (128 MHz, DMSO-d<sub>6</sub>)  $\delta$  (ppm) = -0.36. <sup>19</sup>F NMR (376 MHz, DMSO-d<sub>6</sub>)  $\delta$  -140.95, -141.01. FT-IR ( $\upsilon$  cm<sup>-1</sup>) = 568, 645, 740, 767, 880, 952, 1042, 1102, 1248, 1278, 1322, 1372, 1407, 1429, 1443, 1466, 1569, 1609, 1643, 3123, 3383, 3492. UV/Vis (CH<sub>2</sub>Cl<sub>2</sub>)  $\lambda_{abs}$  (nm) = 456, 477, Fluorescence (CH<sub>2</sub>Cl<sub>2</sub>) (5µM)  $\lambda_{em}$  (nm) = 504. MS (ESI) m/z: [M+H]<sup>+</sup> calculated for C<sub>11</sub>H<sub>10</sub>BF<sub>2</sub>N<sub>3</sub>O<sub>2</sub> 266.0912, found 266.0908.

Section 1: NMR spectrum of synthesized compounds



Figure S2: <sup>13</sup>C-NMR spectra of compound 1 in DMSO-d<sub>6</sub>.



Figure S3: <sup>11</sup>B-NMR spectra of compound 1 in DMSO-d<sub>6</sub>.



Figure S4: <sup>19</sup>F-NMR spectra of compound 1 in DMSO-d<sub>6</sub>.



Figure S5: <sup>1</sup>H-NMR spectra of compound 2 in DMSO-d<sub>6</sub>.



Figure S6: <sup>1</sup>H-<sup>1</sup>H COSY Spectra for compound 2 in DMSO-d<sub>6</sub>.



Figure S7: <sup>13</sup>C-NMR spectra of compound 2 in DMSO-d<sub>6</sub>.



Figure S8: <sup>11</sup>B-NMR spectra of compound 2 in DMSO-d<sub>6</sub>.



Figure S9: <sup>19</sup>F-NMR spectra of compound 2 in DMSO-d<sub>6</sub>.



Figure S10: <sup>1</sup>H-NMR spectra of compound 3 in DMSO-d<sub>6</sub>.



Figure S11: <sup>13</sup>C-NMR spectra of compound 3 in DMSO-d<sub>6</sub>.



Figure S12: <sup>11</sup>B-NMR spectra of compound 3 in DMSO-d<sub>6</sub>.



Figure S13: <sup>19</sup>F-NMR spectra for compound 3 in DMSO-d<sub>6</sub>.



Figure S14: <sup>1</sup>H-NMR spectra of compound 4 in DMSO-d<sub>6</sub>.



Figure S15: <sup>13</sup>C-NMR spectra of compound 4 in DMSO-d<sub>6</sub>.



Figure S16: <sup>11</sup>B-NMR spectra of compound 4 in DMSO-d<sub>6</sub>.





Figure S18: <sup>1</sup>H-NMR spectra of compound 5 in DMSO-d<sub>6</sub>.



Figure S19: <sup>13</sup>C-NMR spectra of compound 5 in DMSO-d<sub>6</sub>.



Figure S20: <sup>11</sup>B-NMR spectra of compound 5 in DMSO-d<sub>6</sub>.



Figure S21: <sup>19</sup>F-NMR spectra of compound 5 in DMSO-d<sub>6</sub>.



Section 2: Mass spectrometry for synthesized compounds

Figure S22: MS of compound 1



Figure S23: MS for compound 2.



Figure S24: MS for compound 3.



Figure S25: MS for compound 4.



Figure S26: MS for compound 5.

# Section 3: Single crystal XRD data

The data was collected at 300K on Bruker D8 QUEST diffractometer with graphite monochromated Mo-*K* $\alpha$  radiation ( $\lambda = 0.71073$  Å) and PHOTON II detector. The structures were refined using SHELXL2019/3<sup>4</sup> and CIF files were deposited in CCDC (<u>2388456</u> and <u>2388457</u>).

Compound	2	4
Empirical Formula	$2(C_{12}H_9BF_2N_2O_3) \cdot 3(H_2O)$	$C_{11}H_8BF_2N_3O_4$
Molecular Weight	610.09	295.01
Crystal Lattice	Orthorhombic	Triclinic
Space Group	$Pca2_1$	$P\overline{1}$
Crystal size (mm <sup>-1</sup> )	$0.21 \times 0.15 \times 0.03$	$0.32 \times 0.08 \times 0.07$
R-factor [%]	4.42	5.51
R <sub>int</sub>	0.086	0.078
$wR_2$	0.1391	0.163
$\mathbf{R}_1$	0.0442	0.055
GooF, S	1.072	1.02
a [Å]	19.7798 (8)	7.2469 (3)
b [Å]	6.9614 (3)	7.8596 (4)
c [Å]	20.1643 (8)	11.2611 (6)
α [°]	90	92.953 (3)
β [°]	90	90.580 (2)
γ [°]	90	108.407 (2)
Cell Volume, V [Å <sup>3</sup> ]	2776.5 (2)	607.55 (5)
F000	1256	300
heta [°]	2.3–24.2°	2.7–21.4°
Z	4	2
T [K]	300	300
$\rho [mg m^{-3}]$	1.459	1.613
No. of Unique reflections	6917	2683
measured		
No. of l. s. parameters	458	196

 Table S1: Summary of crystallographic data for 2 and 4.



Figure S27: ORTEP plots of (A) compound 2 and (B) compound 4 at 50% probability level.

**Table S2:** Bond lengths (Å) and bond angles (deg,  $^{\circ}$ ) of intermolecular hydrogen bonding interactions in compound **4**.

D—H···A	<i>D</i> —Н (Å)	H···A (Å)	$D \cdots A$ (Å)	$D - H \cdots A$ (°)	Symmetry codes
N1—H1…F2	0.81 (3)	2.07 (3)	2.848 (3)	160 (3)	-x+2, -y+1, -z+1
N3—H3…O1	1.00 (3)	2.54 (3)	3.160 (4)	120 (2)	x, y-1, z-1
С3—Н3А…О4	0.93	2.63	3.256 (4)	125	x-1, y-1, z-1
C4—H4…F1	0.93	2.32	3.242 (4)	169	x−1, y, z
C6—H6…F1	0.93	2.50	3.418 (3)	172	x-1, y, z

# Section 4: Computational data



**Figure S28:** Optimized geometries along with molecular orbitals, HOMO-1, HOMO, LUMO, and LUMO+1 for compounds **1-5**.

**Table S3:** Cartesian coordinates of the optimized geometries of compounds **1-5** in the isolated state with their total energies represented as E (in eV).

1 E 24742.020245550 N
E = -24/42.929345550  eV
C, 0.1282025941, 1.8868512863, -0.2146731104
0, 1.3440855194, 1.6449716798, 0.2051539878
C, -0.6850174659, 0.8808007595, -0.739484113
H, -1.6842855272, 1.1046913914, -1.082975991
C, -0.2081037332, -0.431201521, -0.747503408
0, 0.9993638864, -0.7309075143, -0.341159127
C, -0.9958742272, -1.557968925, -1.176054091
C, -2.3098475796, -1.688427804, -1.630061079
N, -0.4388/66257, -2.820003365, -1.178277825
C, -2.5290957736, -3.052254749, -1.905949431
H, -3.0225849477, -0.884323615, -1.743370189
C, -1.3491255024, -3.7276532156, -1.61508621
H, 0.5135096923, -2.9909833097, -0.889689908
H, -3.4395100681, -3.5022120664, -2.27426378
H, -1.1050001/32, -4.7/6857/361, -1.69109108
C, -0.2975360111, 3.2549547017, -0.069680955
C, -1.4963334679, 3.9170749104, -0.342010384
N, 0.5/8/191617, 4.19367/9876, 0.4342979557
C, -1.3215095821, 5.2704223374, 0.007400495
H, -2.3911950701, 3.4049097485, -0.744732081
C, -0.0234380935, 5.409382182, 0.4838503022
$\begin{array}{c} \text{H}, 1.5218774505, 5.9000797505, 0.7089574719} \\ \text{H}, 2.0517796519, 6.0621517977, 0.075276692} \end{array}$
H 0 4002270778 6 2806512025 0 8517666222
R = 2.0420157070 = 0.22000515055, 0.8517000552
$F_{2}$ $87608803 \ 0 \ 1771384875 \ 1 \ 1011017738$
$F_{2} = 67093051/3 = 0.037005233 = 1.1011017736$
<b>7</b>
E = -278267195/1323 eV
$C = 1.2088240557 \pm 0.0392553511 \pm 0.005632229$
0, 1, 2000240337, -0.0392333311, -0.003032227
$C_{0.0164972361} = 0.7482205585 = 0.0960531715$
H $0.0192984235 - 1.8235769078 - 0.195479998$
C = 1.191731306 = 0.0445839776 = 0.0048687586
$O_{\rm c}$ -1 2197110604 1 2548630576 -0 1222447808
C2.47844986640.68423872630.011713031
C2.8806897749. 2.0213938227. 0.0492790065
N3.6244015806, 0.0806391185, -0.0930047139
C4.28689470322.0425335764. 0.0046241115
H, -2.2242480976, -2.8769601507, 0.1162061535
C, -4.7174913901, -0.7223180315, -0.0838343726
H, -3.6010847647, 1.0888359099, -0.1470266688
H, -4.9249390903, -2.9136661005, 0.0323523403
H, -5.7156778108, -0.3137739176, -0.1385367359
C, 2.5088686303, -0.6818050395, -0.0115645683

C. 2.8950995354, -2.0288768833, 0.0493718095
N. 3 6456129068, 0 0707114441, -0 089624952
C = 4.2958746696 - 2.0635968283 = 0.0068674345
H 2 2280466486 $-2.8760926221, 0.1141384227$
C = 4.7440285036 = 0.7402304703 = 0.0707584268
C, 4.7440265050, -0.7402594705, -0.0797564206
$\begin{array}{c} \text{I}, 5.0754987480, 1.080775014, -0.1450212015 \\ \text{I}, 4.0282171701, -2.0208400064, 0.0240154507 \\ \end{array}$
H, 4.9283171701, -2.9398400964, 0.0340154507
B, 0.0126408023, 2.1300859149, 0.040215777
F, 0.0090286747, 2.6448449908, 1.3072726651
F, 0.0065533687, 3.0601637632, -0.9535863193
C, 6.0858329856, -0.1806315739, -0.1529608483
H, 6.9062594209, -0.925803221, -0.1369338657
O, 6.3040892162, 1.0187030342, -0.2269557251
3
E = -25033.2506461  eV
C. 1.21030574520.10342988610.014629139
0, 1, 2294626227, 1, 2389052512, -0, 0606045406
$C_{-0.000336758-0.8142860673-0.0186394444}$
C, -0.000350750, -0.0142000075, 0.0100374444
$G_{1} = 0.0011303002, -1.09419095, 0.0373070094$
$C_{1} = 1.2155290275, -0.1025187250, -0.0121585211$
0, -1.227/570056, 1.2397132034, -0.0576243358
C, -2.5160451211, -0.70878946, -0.0068407733
C, -2.9528248702, -2.049542238, 0.0228594476
N, -3.6546136389, 0.0978339458, -0.0339317417
C, -4.3726773871, -2.0341552911, 0.013638748
H, -2.319061309, -2.9247934622, 0.0478482246
C, -4.778882874, -0.6875447929, -0.0219442629
H, -3.5995971689, 1.1102057087, -0.0579510054
H5.0305520865, -2.890561323, 0.0306477494
H5.7722247844, -0.2641844919, -0.0383058095
$C_{2}$ 5148585195 -0 7104434179 -0 0116330829
C = 2.955148247 = 2.0482128251 = 0.0173133538
N 3 $6407672416$ 0 $1015246855 = 0.0411254173$
C = 4.2752608011 = 2.0242770282 = 0.0054706723
C, 4.5752008011, -2.0542779562, 0.0054700755
H, 2.520970849, -2.927297175, 0.045009855
C, 4.753795539, -0.6869288763, -0.0311408829
H, 3.5934552687, 1.1144295568, -0.0650891888
H, 5.0364084476, -2.8871873325, 0.0212668282
B, 0.0010941877, 2.1232139137, -0.0045567928
F, 0.002591918, 2.8292666168, 1.2192117551
F, -0.0002793571, 2.9773567272, -1.1242061171
I, 6.7088075143, 0.11497676, -0.0665499374
4
E = -30307.541961478 eV
C. 1.17982936830.01651664810.0544063445
0.12079644708.12839492378 - 0.1606266132
C = 0.0016182827 = 0.7361702032 = 0.0638605837
H $0.0112826828 - 1.812/385052 0.1521665216$
$\begin{array}{c} 11, 0.0112020020, -1.01243033333, 0.1321003210 \\ C = 1.2180855356 - 0.0202262505 - 0.0050000602 \end{array}$
$C_{1}$ -1.21070333300, -0.03723033003, -0.00307770003
LU - L / TOTI / YOY4 L / OUUY/YADD -U LU/b /43999

C, -2.498658445, -0.688841506, 0.0061928903
C, -2.8876836791, -2.0309257392, 0.0620400749
N, -3.6534147376, 0.0660334534, -0.0465760526
C, -4.2933322846, -2.0649096494, 0.0430525415
H2.2227730418, -2.8812521338, 0.1087646135
C -4 7376947477 -0 7473765366 -0 0247732904
H -3 6418413996 1 0749501606 -0 0916512784
H -4 9228056448 -2 9420630508 0 0742824058
H -5 7406889193 -0 3482588186 -0 0571010297
C = 2.4868470291 = 0.6483317803 = 0.0924046424
C = 2.89407442 = 1.9891311257 = 0.0529111376
N 3 6102131785 0 1260650616 0 1858122062
C = 4.2056521264 = 2.0128284666 = 0.1220200181
C, 4.2920251204, -2.0126264000, -0.1229290181
H, 2.2403903425, -2.8402191000, 0.0103183097
C, 4.0984/49459, -0.6862283468, -0.2043458522
H, 3.6306590783, 1.1370080696, -0.2315698133
H, 4.9546344572, -2.8676343693, -0.1183644533
B, -0.0275076715, 2.1449824028, 0.0379857584
F, -0.007429149, 2.6444449254, 1.309868888
F, -0.0609800071, 3.0828720399, -0.9463845512
N, 6.0086244974, -0.1302156621, -0.2980609994
O, 6.9572264316, -0.9157274741, -0.310689586
O, 6.0878033264, 1.1031936693, -0.3596406008
5
E = -26249.31876976 eV
C, 1.1860962221, -0.0258577593, -0.0405590408
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4 316514336, -2.0607951172, 0.0545195136
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715
C, $1.1860962221$ , $-0.0258577593$ , $-0.0405590408$ O, $1.1924004516$ , $1.2755167475$ , $-0.2147745755$ C, $-0.0128349912$ , $-0.7395870608$ , $0.0974871343$ H, $-0.0008404555$ , $-1.8101702044$ , $0.2424598321$ C, $-1.2175260517$ , $-0.0568179298$ , $-0.0310124966$ O, $-1.2666519096$ , $1.243892943$ , $-0.2021261531$ C, $-2.5065676905$ , $-0.7050414399$ , $-0.0104241248$ C, $-2.9070531685$ , $-2.0376785589$ , $0.0912794459$ N, $-3.6520963674$ , $0.0560496833$ , $-0.1079405444$ C, $-4.316514336$ , $-2.0607951172$ , $0.0545195136$ H, $-2.249556336$ , $-2.8906785581$ , $0.1782927634$ C, $-4.748391975$ , $-0.746160433$ , $-0.0699555477$ H, $-3.6243865992$ , $1.061738531$ , $-0.1924591715$ H $-4.95317915$ , $-2.9318535379$ , $0.1105625075$
C, $1.1860962221$ , $-0.0258577593$ , $-0.0405590408$ O, $1.1924004516$ , $1.2755167475$ , $-0.2147745755$ C, $-0.0128349912$ , $-0.7395870608$ , $0.0974871343$ H, $-0.0008404555$ , $-1.8101702044$ , $0.2424598321$ C, $-1.2175260517$ , $-0.0568179298$ , $-0.0310124966$ O, $-1.2666519096$ , $1.243892943$ , $-0.2021261531$ C, $-2.5065676905$ , $-0.7050414399$ , $-0.0104241248$ C, $-2.9070531685$ , $-2.0376785589$ , $0.0912794459$ N, $-3.6520963674$ , $0.0560496833$ , $-0.1079405444$ C, $-4.316514336$ , $-2.0607951172$ , $0.0545195136$ H, $-2.249556336$ , $-2.8906785581$ , $0.1782927634$ C, $-4.748391975$ , $-0.746160433$ , $-0.0699555477$ H, $-3.6243865992$ , $1.061738531$ , $-0.1924591715$ H, $-4.95317915$ , $-2.9318535379$ , $0.1105625075$
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715 H, -4.95317915, -2.9318535379, 0.1105625075 H, -5.7462161665, -0.3379686381, -0.1319153407
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715 H, -4.95317915, -2.9318535379, 0.1105625075 H, -5.7462161665, -0.3379686381, -0.1319153407 C, 2.4768892337, -0.6346740225, -0.0310399325
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715 H, -4.95317915, -2.9318535379, 0.1105625075 H, -5.7462161665, -0.3379686381, -0.1319153407 C, 2.4768892337, -0.6346740225, -0.0310399325 C, 2.9233232258, -1.9519494098, 0.0845982057
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715 H, -4.95317915, -2.9318535379, 0.1105625075 H, -5.7462161665, -0.3379686381, -0.1319153407 C, 2.4768892337, -0.6346740225, -0.0310399325 C, 2.9233232258, -1.9519494098, 0.0845982057 N, 3.6129298329, 0.1622897277, -0.155703312
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715 H, -4.95317915, -2.9318535379, 0.1105625075 H, -5.7462161665, -0.3379686381, -0.1319153407 C, 2.4768892337, -0.6346740225, -0.0310399325 C, 2.9233232258, -1.9519494098, 0.0845982057 N, 3.6129298329, 0.1622897277, -0.155703312 C, 4.3268617638, -1.9437533254, 0.0355772896
C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715 H, -4.95317915, -2.9318535379, 0.1105625075 H, -5.7462161665, -0.3379686381, -0.1319153407 C, 2.4768892337, -0.6346740225, -0.0310399325 C, 2.9233232258, -1.9519494098, 0.0845982057 N, 3.6129298329, 0.1622897277, -0.155703312 C, 4.3268617638, -1.9437533254, 0.0355772896 H, 2.2932328407, -2.8217506782, 0.2034352242
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C, 1.1860962221, -0.0258577593, -0.0405590408 O, 1.1924004516, 1.2755167475, -0.2147745755 C, -0.0128349912, -0.7395870608, 0.0974871343 H, -0.0008404555, -1.8101702044, 0.2424598321 C, -1.2175260517, -0.0568179298, -0.0310124966 O, -1.2666519096, 1.243892943, -0.2021261531 C, -2.5065676905, -0.7050414399, -0.0104241248 C, -2.9070531685, -2.0376785589, 0.0912794459 N, -3.6520963674, 0.0560496833, -0.1079405444 C, -4.316514336, -2.0607951172, 0.0545195136 H, -2.249556336, -2.8906785581, 0.1782927634 C, -4.748391975, -0.746160433, -0.0699555477 H, -3.6243865992, 1.061738531, -0.1924591715 H, -4.95317915, -2.9318535379, 0.1105625075 H, -5.7462161665, -0.3379686381, -0.1319153407 C, 2.4768892337, -0.6346740225, -0.0310399325 C, 2.9233232258, -1.9519494098, 0.0845982057 N, 3.6129298329, 0.1622897277, -0.155703312 C, 4.3268617638, -1.9437533254, 0.0355772896 H, 2.2932328407, -2.8217506782, 0.2034352242 C, 4.7277804492, -0.6089478559, -0.1174600601 H, 3.5542890799, 1.1599353562, -0.3005475249
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C, $1.1860962221$ , $-0.0258577593$ , $-0.0405590408$ O, $1.1924004516$ , $1.2755167475$ , $-0.2147745755$ C, $-0.0128349912$ , $-0.7395870608$ , $0.0974871343$ H, $-0.0008404555$ , $-1.8101702044$ , $0.2424598321$ C, $-1.2175260517$ , $-0.0568179298$ , $-0.0310124966$ O, $-1.2666519096$ , $1.243892943$ , $-0.2021261531$ C, $-2.5065676905$ , $-0.7050414399$ , $-0.0104241248$ C, $-2.9070531685$ , $-2.0376785589$ , $0.0912794459$ N, $-3.6520963674$ , $0.0560496833$ , $-0.1079405444$ C, $-4.316514336$ , $-2.0607951172$ , $0.0545195136$ H, $-2.249556336$ , $-2.8906785581$ , $0.1782927634$ C, $-4.748391975$ , $-0.746160433$ , $-0.0699555477$ H, $-3.6243865992$ , $1.061738531$ , $-0.1924591715$ H, $-4.95317915$ , $-2.9318535379$ , $0.1105625075$ H, $-5.7462161665$ , $-0.3379686381$ , $-0.1319153407$ C, $2.4768892337$ , $-0.6346740225$ , $-0.0310399325$ C, $2.9233232258$ , $-1.9519494098$ , $0.0845982057$ N, $3.6129298329$ , $0.1622897277$ , $-0.155703312$ C, $4.3268617638$ , $-1.9437533254$ , $0.0355772896$ H, $2.2932328407$ , $-2.8217506782$ , $0.2034352242$ C, $4.7277804492$ , $-0.6089478559$ , $-0.1174600601$ H, $3.5542890799$ , $1.1599353562$ , $-0.3005475249$ H, $4.9904527101$ , $-2.7935526143$ , $0.1045767487$ B, $-0.0485123803$ , $2.1233218118$ , $-0.0450122928$

F, -0.063621869, 3.0630400213, -1.0364495101	
N, 5.9930115505, -0.0762964847, -0.2858756499	
H, 6.1334130325, 0.8480764971, 0.1020879995	
H, 6.7378807213, -0.7060873416, -0.0219098904	

**Table S4:** HOMO to LUMO orbital contributions from  $S_0 \rightarrow S_1$  state along with the corresponding oscillator strengths obtained from TD-B3LYP/6-31G+(d,p) in dichloromethane

Compound	Functional	Main orbital transition	$\lambda_{\max}$	ΔΕ	f
	group	$\mathbf{S}_0 \to \mathbf{S}_1$	(nm)	( <b>eV</b> )	
1	-H	HOMO $\rightarrow$ LUMO (100%)	374	3.316	1.5372
2	-CHO	HOMO $\rightarrow$ LUMO (100%)	394	3.148	1.6406
3	-I	HOMO $\rightarrow$ LUMO (100%)	399	3.106	1.7897
4	$-NO_2$	HOMO $\rightarrow$ LUMO (47.36%)	427	2.905	1.1335
5	$-NH_2$	HOMO $\rightarrow$ LUMO (100%)	399	3.107	1.6908





**Figure S29:** Time-resolved fluorescence decay profiles for compounds (A) **4** (B) **5** in CH<sub>2</sub>Cl<sub>2</sub> solvent.



Figure S30: Time-resolved fluorescence decay profile for compound 2 in different solvents.

Solvents	$\lambda_{em}$ (nm)	τ (ns)	X <sup>2</sup>
THF	464	1.00, 3.57	1.375
EtOAc	460	0.81, 2.84	1.330
DMF	475	0.51, 2.77	1.605
DMSO	487	0.42, 4.00	1.774
ACN	467	0.41, 2.15	1.580

**Table S5:** TCSPC studies for compound 2 in different solvents.



**Figure S31:** Comparison of the photostabilities of compounds (A) **2**, (B) **3**, (C) **4**, (D) **5** in acetonitrile  $(5 \times 10^{-6} \text{ M})$  under continuous UV irradiation (319 nm) over 3 h.



**Figure S32:** Change of optical density of compounds **2-5** at the absorption maximum wavelength ( $\lambda_{max}$ ) in acetonitrile (5×10<sup>-6</sup> M) under UV irradiation (319 nm) over 3 h.



**Figure S33:** Normalized absorption spectra of compounds (A) **1**, (B) **2**, (C) **3**, (D) **4** and (E) **5** in various solvents.

Solvent	Dielectric	Refractive	λabs	λemi	Stokes shift
	constant (ɛ)	index (ŋ)	(nm)	(nm)	(cm <sup>-1</sup> )
1		> <b>*</b> /			
DCM	8.93	1.424	432	451	975
THF	7.58	1.407	431	446	780
EtOAc	6.02	1.372	429	444	787
DMF	36.70	1.430	437	455	905
DMSO	46.70	1.479	441	460	937
ACN	35.94	1.344	431	450	980
2					
DCM	8.93	1.424	427, 447	467	958
THF	7.58	1.407	426, 445	464	920
EtOAc	6.02	1.372	424, 442	460	885
DMF	36.70	1.430	432, 451	475	1120
DMSO	46.70	1.479	435, 455	487	1444
ACN	35.94	1.344	424, 444	467	1109
3					
DCM	8.93	1.424	437	457	1001
THF	7.58	1.407	436	452	812
EtOAc	6.02	1.372	433	449	823
DMF	36.70	1.430	443	462	928
DMSO	46.70	1.479	447	466	912
ACN	35.94	1.344	435	456	1059
4					
DCM	8.93	1.424	436, 452	502	2202
THF	7.58	1.407	454, 475	496	1865
EtOAc	6.02	1.372	434, 451	490	1765
DMF	36.70	1.430	460, 481	503	909
DMSO	46.70	1.479	462, 484	510	1053
ACN	35.94	1.344	452, 475	503	1171
5					
DCM	8.93	1.424	456, 477	504	1123
THF	7.58	1.407	460, 481	505	988
EtOAc	6.02	1.372	460, 481	499	750
DMF	36.70	1.430	467, 490	516	1028
DMSO	46.70	1.479	470, 496	521	967
ACN	35.94	1.344	460, 480	508	1148

**Table S6**: Experimental photophysical properties of compounds 1-5 in various solvents.





# Section 6: Electrochemical studies



**Figure S34:** Electrochemical redox data of compounds **1-5** (blue - oxidation, red - reduction) in acetonitrile containing 0.1 M tetrabutylammonium perchlorate as a supporting electrolyte recorded at a scan rate of 100 mV/sec (**1** and **2**), 50 mV/sec (**3**, **4** and **5**).

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