Supporting Information

Structural insight into imidazopyridines and benzimidazoles: the importance of hydrogen bond, π-stacking interactions and intramolecular charge transfer effect for fluorescence

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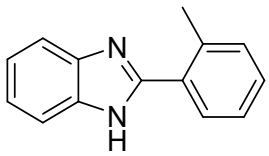
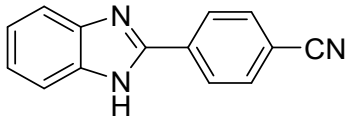
1. Experimental Characterization Data for the Products



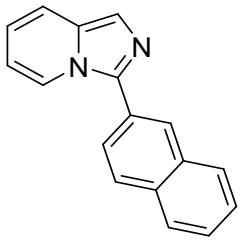
2-(o-tolyl)-1H-benzo[d]imidazole (2a):

From benzene-1,2-diamine (1 mmol, 1 eq.) and 2-methylbenzaldehyde (1.75 mmol, 1.75 eq.), following the general procedure C, the title compound (174.7 mg, 84%) was obtained as a faint yellow solid. Rf = 0.3 (petroleum ether/ethyl acetate = 20:1 - 5:1). ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.82-7.73 (m, 1H), 7.63 (s, 2H), 7.39 (s, 3H), 7.22 (s, 2H), 2.62 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ: 152.41, 137.49, 131.72, 130.53, 129.92, 129.78, 126.42, 122.35, 21.50.



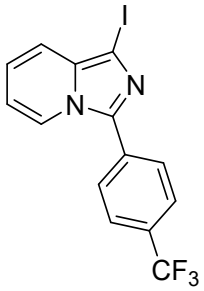
4-(1H-benzo[d]imidazol-2-yl)benzonitrile (2b):

From benzene-1,2-diamine (1 mmol, 1 eq.) and 4-formyl benzonitrile (1.75 mmol, 1.75 eq.), following the general procedure C, the title compound (210.2 mg, 96%) was obtained as a faint yellow solid. Rf = 0.3 (petroleum ether/ethyl acetate = 20:1 - 5:1). ^{1}H NMR (400 MHz, DMSO-d_6) δ: 8.34 (d, *J* = 7.6 Hz, 2H), 8.01 (d, *J* = 7.3 Hz, 2H), 7.65 (s, 2H), 7.32-7.20 (m, 2H); ^{13}C NMR (101 MHz, DMSO-d_6) δ: 149.83, 136.47, 134.71, 133.40, 133.24, 133.19, 130.27, 127.56, 127.43, 123.27, 119.08, 112.35.



3-(naphthalen-2-yl)imidazo[1,5-a]pyridine (3a):

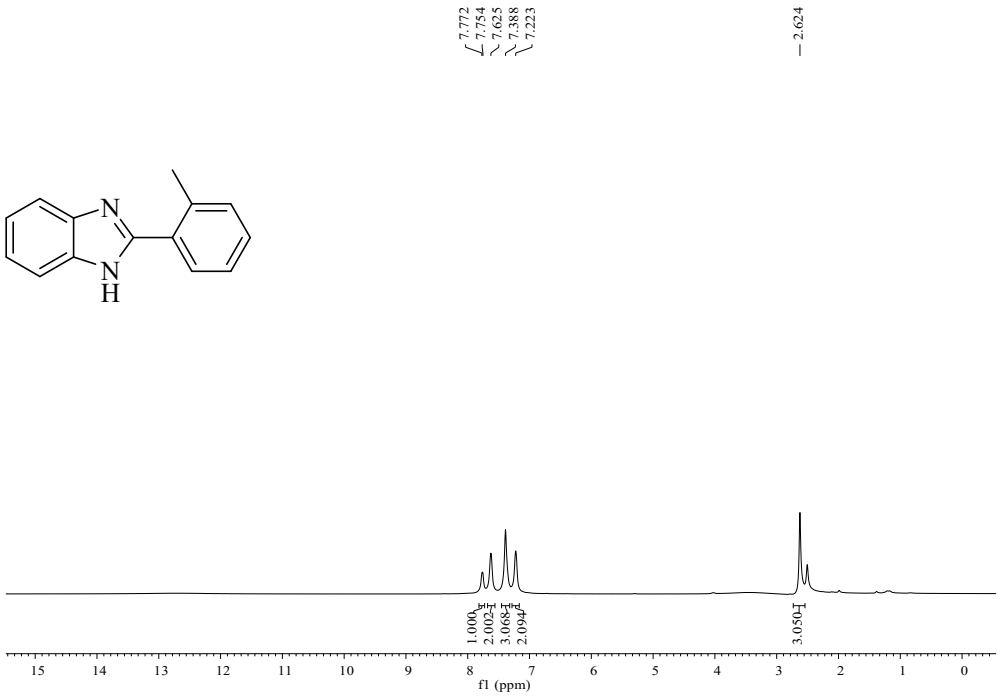
From 2-pyridinemethanamine (0.8 mmol, 2 eq.) and 2-naphthaldehyde (0.4 mmol, 1 eq.), following the general procedure A, the title compound (71.2 mg, 73%) was obtained as a faint yellow solid. Rf = 0.3 (petroleum ether/ethyl acetate = 20:1 - 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.41 (d, *J* = 7.3 Hz, 1H), 8.29 (s, 1H), 8.04-7.91 (m, 4H), 7.64 (s, 1H), 7.58-7.52 (m, 3H), 6.82-6.73 (m, 1H), 6.62 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 138.28, 133.37, 133.15, 131.83, 128.81, 128.24, 127.85, 126.69, 126.66, 126.63, 125.72, 121.51, 120.96, 118.91, 113.25.



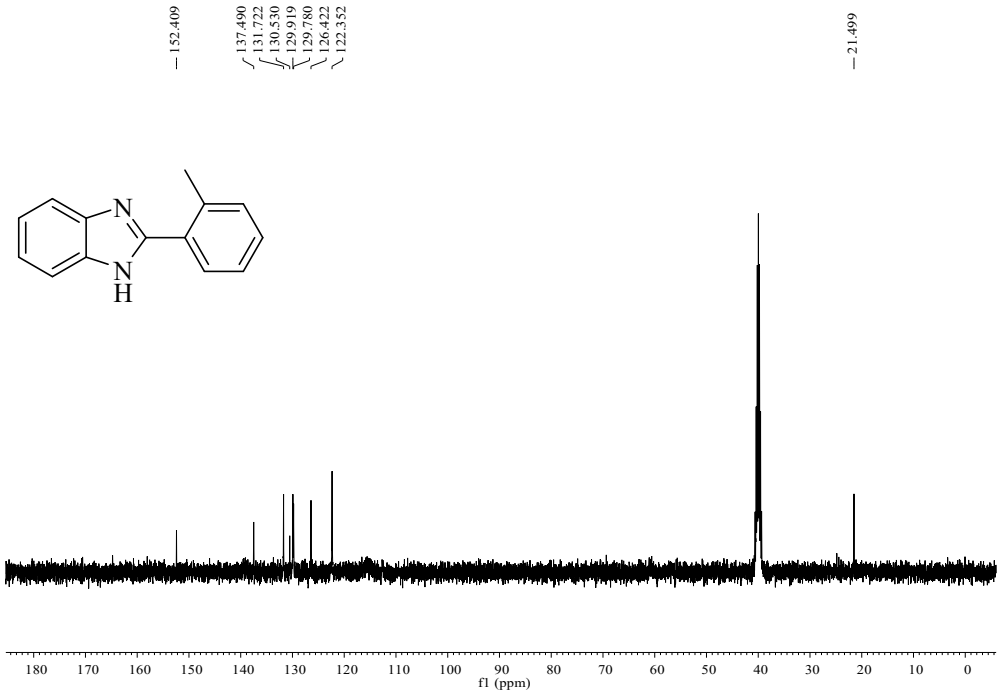
1-iodo-3-(4-(trifluoromethyl)phenyl)imidazo[1,5-a]pyridine (3b):

From 2-pyridinemethanamine (0.8 mmol, 1 eq.) and 4-(trifluoromethyl)benzaldehyde (1.6 mmol, 2 eq.), following the general procedure B, the title compound (304.2 mg, 98%) was obtained as a faint yellow solid. Rf = 0.3 (petroleum ether/ethyl acetate = 15:1 – 3:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.09 (d, *J* = 7.3 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 9.2 Hz, 1H), 6.71 (dd, *J* = 9.3, 6.4 Hz, 1H), 6.54 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 138.74, 133.98, 132.72, 130.48 (d, *J* = 32.6 Hz), 127.80, 125.94 (q, *J* = 3.8 Hz), 123.90 (d, *J* = 272.3 Hz), 121.56, 120.83, 119.10, 114.71, 75.11; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.61.

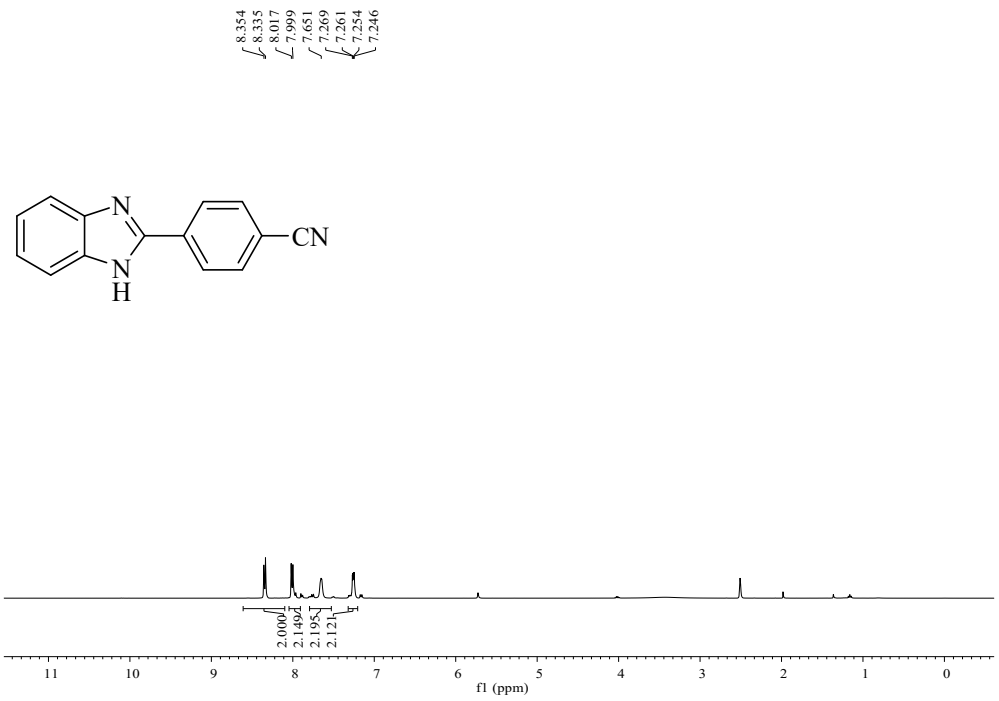
Copies of NMR Spectra for Compounds



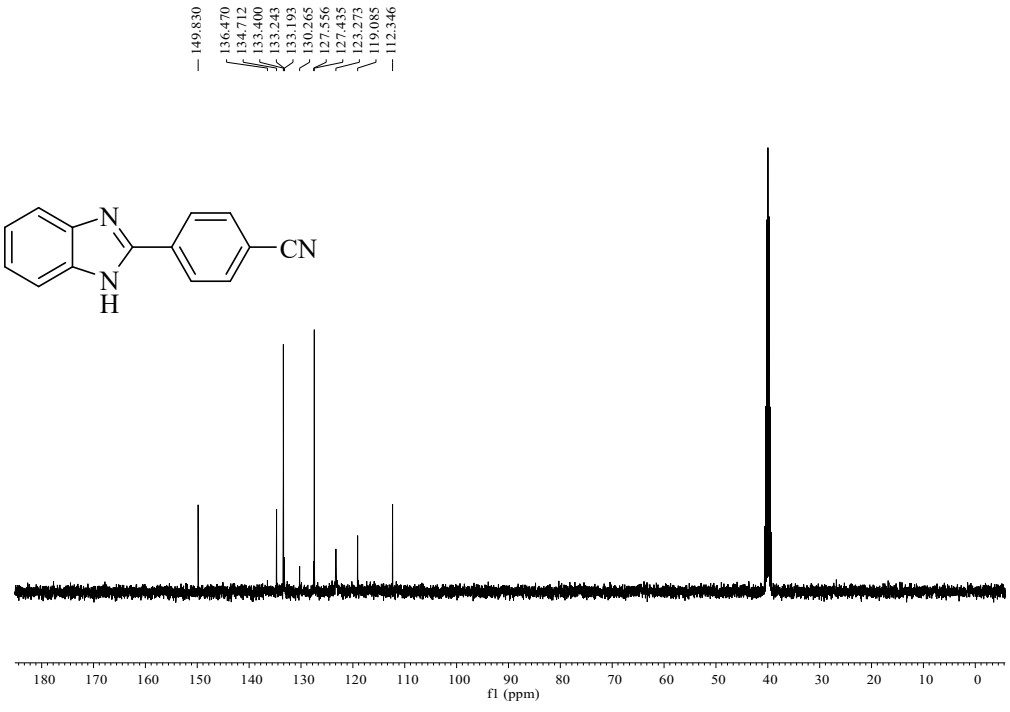
^{1}H NMR Spectrum of **2a**



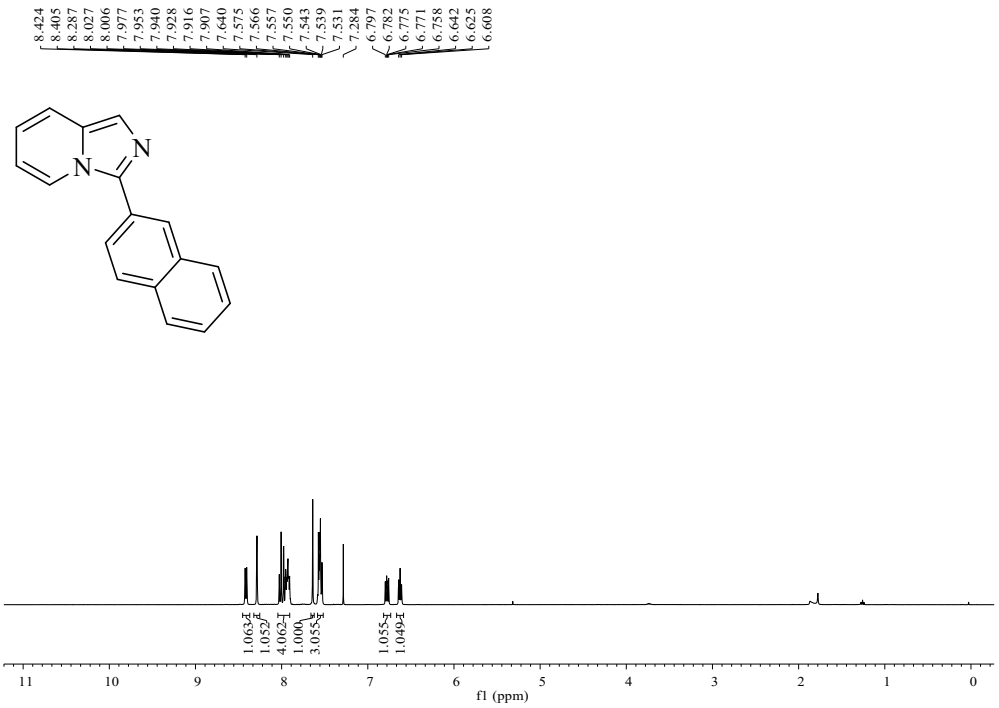
^{13}C NMR Spectrum of **2a**



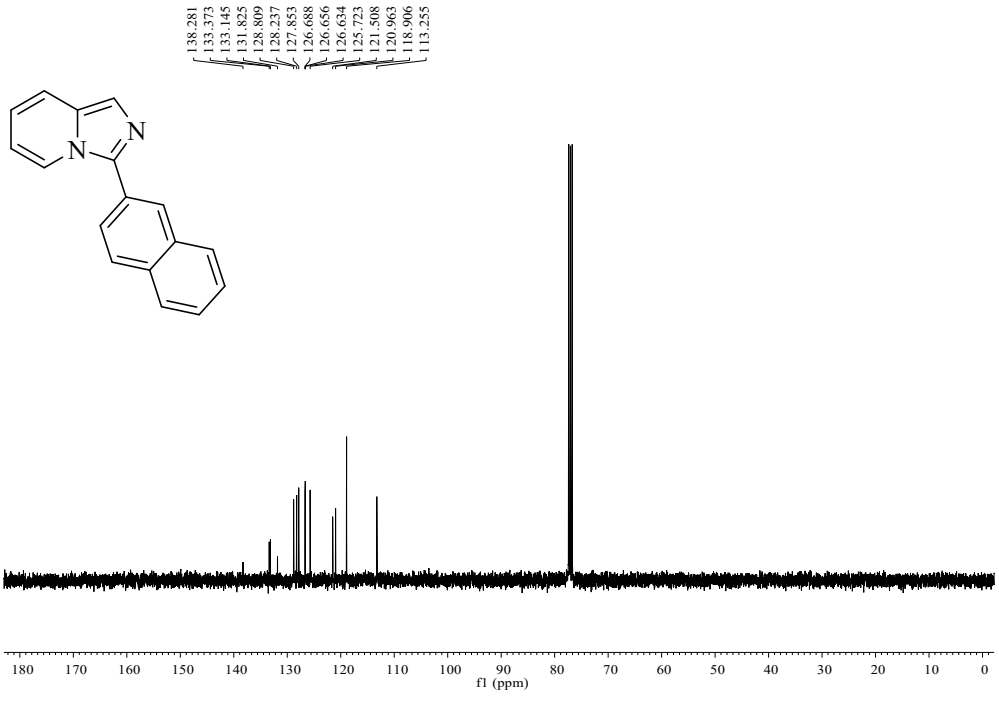
^{1}H NMR Spectrum of **2b**



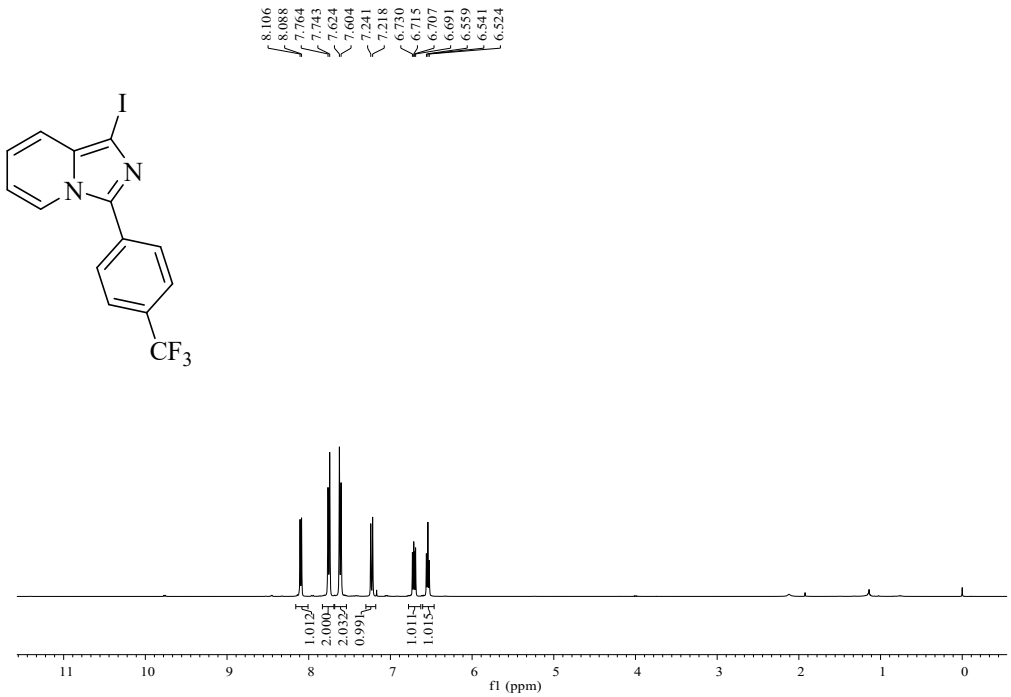
^{13}C NMR Spectrum of **2b**



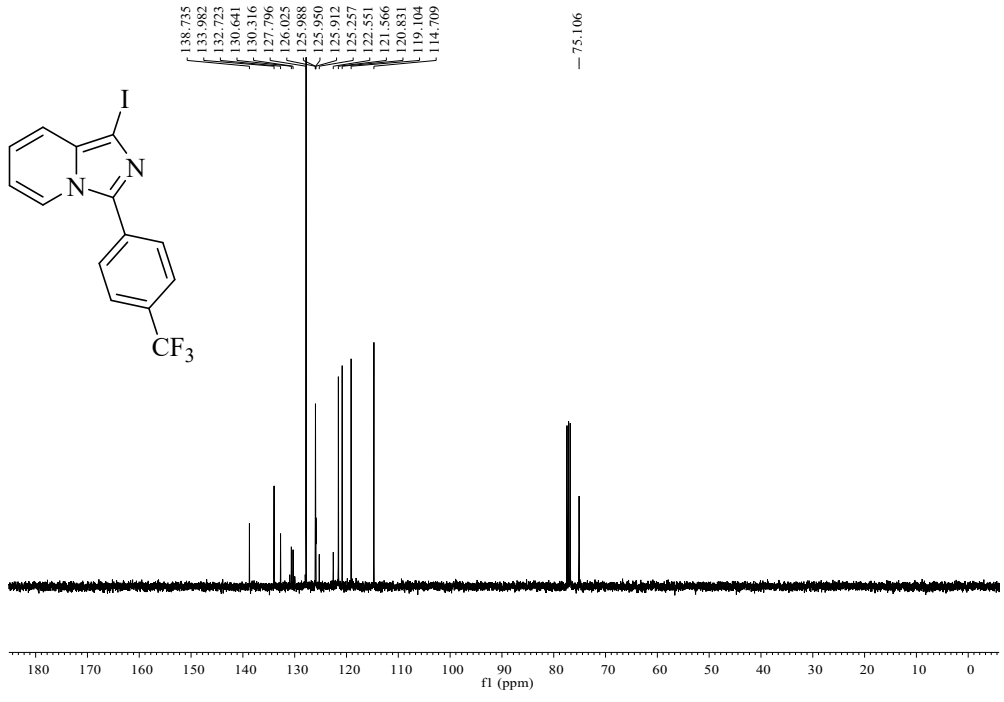
^{1}H NMR Spectrum of **3a**



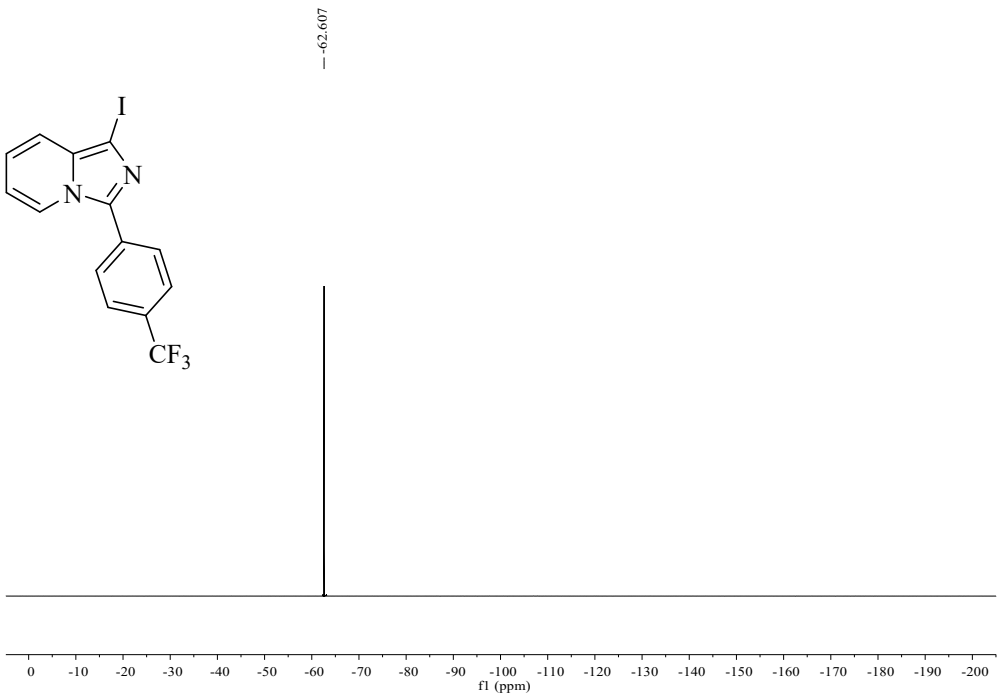
^{13}C NMR Spectrum of **3a**



^{1}H NMR Spectrum of **3b**



^{13}C NMR Spectrum of **3b**



^{19}F NMR Spectrum of **3b**

2. X-ray Crystal Structure Determination of the Products (2a, 2b, 3a, and 3b) and Hirshfeld Surface (HS) Analysis

To grow the crystals used to collect the X-ray data for **2a**, **2b**, **3a**, and **3b** the following method was used: the sample was dissolved with 3 mL CH_3OH in a small vial, which was kept aside at room temperature to obtain crystals.

Table S1. Crystallographic data for compounds **2a**

Project	**Parameter**
Identification code	202210190
Empirical formula	$C_{14}H_{12}N_2$
Formula weight	208.26
Temperature/K	293(2)
Crystal system	tetragonal
Space group	$P4_1$
a/Å	8.8835(11)
b/Å	8.8835(11)
c/Å	14.400(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1136.4(3)
Z	4
ρcalcg/cm^3	1. 217
μ/mm^{-1}	0.568
F(000)	440.0
Crystal size/mm^3	0.22 × 0.09 × 0.07
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.956 to 133.894
Index ranges	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -15 ≤ l ≤ 17
Reflections collected	7582
Independent reflections	1882 [R_{int} = 0.0432, R_{sigma} = 0.0385]
Data/restraints/parameters	1882/1/151
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0392, wR_2 = 0.1048
Final R indexes [all data]	R_1 = 0.0508, wR_2 = 0.1181
Largest diff. peak/hole / e Å^{-3}	0.13/-0.12

Table S2. Bond lengths for single crystal **2a**

Atom	Length/Å	Atom	Length/Å
N(1)-C(6)	1.376(4)	C(5)-C(6)	1.399(5)
N(1)-C(7)	1.369(4)	C(7)-C(8)	1.479(4)
N(2)-C(5)	1.398(4)	C(8)-C(9)	1.386(5)
N(2)-C(7)	1.319(4)	C(8)-C(13)	1.401(6)
C(1)-C(2)	1.379(6)	C(9)-C(10)	1.394(6)
C(1)-C(6)	1.384(5)	C(10)-C(11)	1.378(8)
C(2)-C(3)	1.393(7)	C(11)-C(12)	1.375(8)
C(3)-C(4)	1.371(6)	C(12)-C(13)	1.396(6)
C(4)-C(5)	1.392(5)	C(13)-C(14)	1.498(6)

Table S3. Bond angles for single crystal **2a**

Atom	Angle/°	Atom	Angle/°
C(7)-N(1)-C(6)	107.4(3)	N(2)-C(7)-N(1)	112.5(3)
C(7)-N(2)-C(5)	105.0(3)	N(2)-C(7)-C(8)	126.3(3)
C(2)-C(1)-C(6)	116.6(4)	C(9)-C(8)-C(7)	117.9(3)
C(1)-C(2)-C(3)	122.0(4)	C(9)-C(8)-C(13)	120.2(3)
C(4)-C(3)-C(2)	121.2(4)	C(13)-C(8)-C(7)	121.9(3)
C(3)-C(4)-C(5)	118.1(4)	C(8)-C(9)-C(10)	121.0(5)
N(2)-C(5)-C(6)	109.7(3)	C(11)-C(10)-C(9)	119.2(5)
C(4)-C(5)-N(2)	130.2(3)	C(12)-C(11)-C(10)	119.9(4)
C(4)-C(5)-C(6)	120.0(3)	C(11)-C(12)-C(13)	122.2(5)
N(1)-C(6)-C(1)	132.5(3)	C(8)-C(13)-C(14)	122.9(3)
N(1)-C(6)-C(5)	105.4(3)	C(12)-C(13)-C(8)	117.6(4)
C(1)-C(6)-C(5)	122.2(3)	C(12)-C(13)-C(14)	119.6(4)
N(1)-C(7)-C(8)	121.1(3)		

Table S4. Crystallographic data for compounds **2b**

Project	**Parameter**
Identification code	LQJ-1
Empirical formula	$C_{14}H_9N_3$
Formula weight	219.24
Temperature/K	300.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.2378(10)
b/Å	11.8288(14)
c/Å	12.7296(17)
α/°	90
β/°	92.175(5)
γ/°	90
Volume/Å^3	1089.1(2)
Z	4
ρcalcg/cm^3	1.337
μ/mm^{-1}	0.083
F(000)	456.0
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.374 to 50
Index ranges	-8 ≤ h ≤ 8, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	27964
Independent reflections	1928 [R_{int} = 0.0529, R_{sigma} = 0.0185]
Data/restraints/parameters	1928/0/154
Goodness-of-fit on F^2	1.107
Final R indexes [I>=2σ (I)]	R_1 = 0.0356, wR_2 = 0.0874
Final R indexes [all data]	R_1 = 0.0455, wR_2 = 0.0935
Largest diff. peak/hole / e Å^{-3}	0.10/-0.18

Table S5. Bond lengths for single crystal **2b**

Atom	Length/Å	Atom	Length/Å
N(1)-C(2)	1.3769(18)	C(8)-C(9)	1.391(2)
N(1)-C(7)	1.3670(18)	C(11)-C(14)	1.441(2)
N(2)-C(3)	1.3845(18)	C(11)-C(12)	1.389(2)
N(2)-C(7)	1.3199(18)	C(11)-C(10)	1.386(2)
N(3)-C(14)	1.1424(18)	C(4)-C(5)	1.375(2)
C(2)-C(3)	1.400(2)	C(13)-C(12)	1.375(2)
C(2)-C(1)	1.392(2)	C(1)-C(6)	1.376(2)
C(3)-C(4)	1.398(2)	C(10)-C(9)	1.380(2)
C(7)-C(8)	1.4699(19)	C(5)-C(6)	1.398(2)
C(8)-C(13)	1.393(2)		

Table S6. Bond angles for single crystal **2b**

Atom	Angle/°	Atom	Angle/°
C(7)-N(1)-C(2)	107.17(11)	C(9)-C(8)-C(13)	118.80(13)
C(7)-N(2)-C(3)	104.90(12)	C(12)-C(11)-C(14)	118.74(13)
N(1)-C(2)-C(3)	105.05(12)	C(10)-C(11)-C(14)	121.28(14)
N(1)-C(2)-C(1)	132.56(13)	C(10)-C(11)-C(12)	119.98(13)
C(1)-C(2)-C(3)	122.39(13)	C(5)-C(4)-C(3)	117.93(14)
N(2)-C(3)-C(2)	110.23(12)	N(3)-C(14)-C(11)	177.15(17)
N(2)-C(3)-C(4)	130.01(13)	C(12)-C(13)-C(8)	120.73(14)
C(4)-C(3)-C(2)	119.75(13)	C(13)-C(12)-C(11)	119.94(14)
N(1)-C(7)-C(8)	123.86(12)	C(6)-C(1)-C(2)	116.72(14)
N(2)-C(7)-N(1)	112.64(12)	C(9)-C(10)-C(11)	119.77(14)
N(2)-C(7)-C(8)	123.48(13)	C(10)-C(9)-C(8)	120.78(14)
C(13)-C(8)-C(7)	118.41(13)	C(4)-C(5)-C(6)	121.50(15)
C(9)-C(8)-C(7)	122.79(13)	C(1)-C(6)-C(5)	121.69(14)

Table S7. Crystallographic data for compounds **3a**

Project	Parameter
Identification code	202209166
Empirical formula	$C_{17}H_{12}N_2$
Formula weight	244.29
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.4481(3)
b/Å	12.5608(7)
c/Å	13.0832(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1223.99(12)
Z	4
ρcalcg/cm^3	1.326
μ/mm^{-1}	0.615
F (000)	512.0
Crystal size/mm^3	0.18 × 0.07 × 0.06
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.762 to 141.976
Index ranges	-9 ≤ h ≤ 8, -15 ≤ k ≤ 15, -16 ≤ l ≤ 15
Reflections collected	6812
Independent reflections	2344 [R_{int} = 0.0345, R_{sigma} = 0.0372]
Data/restraints/parameters	2344/0/173
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0401, wR_2 = 0.0968
Final R indexes [all data]	R_1 = 0.0507, wR_2 = 0.1043
Largest diff. peak/hole / e Å^{-3}	0.11/-0.12

Table S8. Bond lengths for single crystal **3a**

Atom	Length/Å	Atom	Length /Å
N(1)-C(1)	1.380(4)	C(8)-C(9)	1.423(4)
N(1)- C(5)	1.400(4)	C(8)- C(13)	1.374(4)
N(1)- C(7)	1.377(3)	C(9)- C(10)	1.358(4)
N(2)- C(6)	1.357(4)	C(10)-C(11)	1.413(5)
N(2)-C(7)	1.324(4)	C(11)-C(12)	1.422(4)
C(1)- C(2)	1.346(4)	C(11)-C(14)	1.416(4)
C(2)- C(3)	1.422(5)	C(12)-C(13)	1.418(4)
C(3)- C(4)	1.347(5)	C(12)-C(17)	1.412(4)
C(4)- C(5)	1.411(4)	C(14)-C(15)	1.353(5)
C(5)- C(6)	1.375(4)	C(15)-C(16)	1.410(5)
C(7)- C(8)	1.464(4)	C(16)-C(17)	1.370(4)

Table S9. Bond angles for single crystal **3a**

Atom	Angle/°	Atom	Angle /°
C(1)-N(1)-C(5)	120.7(3)	C(13)-C(8)-C(7)	122.2(2)
C(7)-N(1)-C(1)	132.0(2)	C(13)-C(8)-C(9)	118.9(3)
C(7)-N(1)-C(5)	107.2(2)	C(10)-C(9)-C(8)	120.7(3)
C(7)-N(2)-C(6)	106.9(3)	C(9)-C(10)-C(11)	121.4(3)
C(2)-C(1)-N(1)	119.8(3)	C(10)-C(11)-C(12)	118.7(3)
C(1)-C(2)-C(3)	120.5(3)	C(10)-C(11)-C(14)	123.1(3)
C(4)-C(3)-C(2)	120.3(3)	C(14)-C(11)-C(12)	118.1(3)
C(3)-C(4)-C(5)	119.8(3)	C(13)-C(12)-C(11)	118.6(3)
N(1)-C(5)-C(4)	118.7(3)	C(17)-C(12)-C(11)	119.3(3)
C(6)-C(5)-N(1)	104.6(3)	C(17)-C(12)-C(13)	122.1(3)
C(6)-C(5)-C(4)	136.7(3)	C(8)-C(13)-C(12)	121.7(2)
N(2)-C(6)-C(5)	111.0(3)	C(15)-C(14)-C(11)	121.3(3)
N(1)-C(7)-C(8)	125.7(2)	C(14)-C(15)-C(16)	120.8(3)
N(2)-C(7)-N(1)	110.2(2)	C(17)-C(16)-C(15)	119.7(3)
N(2)-C(7)-C(8)	123.9(3)	C(16)-C(17)-C(12)	120.7(3
C(9)-C(8)-C(7)	118.7(3)		

Table S10. Crystallographic data for compounds **3b**

Project	**Parameter**
Identification code	202209167
Empirical formula	$C_{14}H_8F_3IN_2$
Formula weight	388.12
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	24.8694(3)
b/Å	7.34027(12)
c/Å	15.1137(2)
α/°	90
β/°	102.0839(13)
γ/°	90
Volume/Å^3	2697.85(7)
Z	8
ρcalcg/cm^3	1.911
μ/mm^{-1}	18.920
F(000)	1488.0
Crystal size/mm^3	0.17 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.27 to 141.938
Index ranges	-30 ≤ h ≤ 30, -7 ≤ k ≤ 8, -18 ≤ l ≤ 16
Reflections collected	10691
Independent reflections	2577 [R_{int} = 0.0424, R_{sigma} = 0.0330]
Data/restraints/parameters	2577/54/191
Goodness-of-fit on F^2	1.102
Final R indexes [I>=2σ (I)]	R_1 = 0.0455, wR_2 = 0.1178
Final R indexes [all data]	R_1 = 0.0494, wR_2 = 0.1224
Largest diff. peak/hole / e Å^{-3}	0.57/-1.70

Table S11. Bond lengths for single crystal **3b**

Atom	Length/Å	Atom	Length/Å
I(1)-C(6)	2.069(4)	C(2)-C(3)	1.425(7)
F(1)-C(14)	1.337(8)	C(3)-C(4)	1.344(7)
F(1A)-C(14)	1.315(14)	C(4)-C(5)	1.416(5)
F(2)-C(14)	1.334(9)	C(5)-C(6)	1.369(6)
F(2A)-C(14)	1.285(14)	C(7)-C(8)	1.462(5)
F(3)-C(14)	1.312(8)	C(8)-C(9)	1.399(5)
F(3A)-C(14)	1.356(14)	C(8)-C(13)	1.388(6)
N(1)-C(1)	1.387(5)	C(9)-C(10)	1.372(6)
N(1)-C(5)	1.403(5)	C(10)-C(11)	1.394(7)
N(1)-C(7)	1.376(4)	C(11)-C(12)	1.383(7)
N(2)-C(6)	1.356(5)	C(11)-C(14)	1.490(6)
N(2)-C(7)	1.333(5)	C(12)-C(13)	1.390(7)
C(1)-C(2)	1.342(6)		

Table S12. Bond angles for single crystal **3b**

Atom	Angle/°	Atom	Angle/°
C(1)-N(1)-C(5)	120.8(3)	C(10)-C(9)-C(8)	121.3(4)
C(7)-N(1)-C(1)	132.0(3)	C(9)-C(10)-C(11)	119.6(4)
C(7)-N(1)-C(5)	106.8(3)	C(10)-C(11)-C(14)	120.1(4)
C(7)-N(2)-C(6)	105.8(3)	C(12)-C(11)-C(10)	120.2(4)
C(2)-C(1)-N(1)	119.2(4)	C(12)-C(11)-C(14)	119.7(5)
C(1)-C(2)-C(3)	121.2(4)	C(11)-C(12)-C(13)	119.5(4)
C(4)-C(3)-C(2)	120.1(4)	C(8)-C(13)-C(12)	121.1(4)
C(3)-C(4)-C(5)	119.8(4)	F(1)-C(14)-C(11)	113.1(5)
N(1)-C(5)-C(4)	118.6(4)	F(1A)-C(14)-F(3A)	96.1(13)
C(6)-C(5)-N(1)	104.6(3)	F(1A)-C(14)-C(11)	113.8(10)
C(6)-C(5)-C(4)	136.9(4)	F(2)-C(14)-F(1)	102.5(6)
N(2)-C(6)-I(1)	122.3(3)	F(2)-C(14)-C(11)	111.5(7)
N(2)-C(6)-C(5)	112.0(3)	F(2A)-C(14)-F(1A)	115.2(17)
C(5)-C(6)-I(1)	125.7(3)	F(2A)-C(14)-F(3A)	103.3(19)
N(1)-C(7)-C(8)	126.2(3)	F(2A)-C(14)-C(11)	118(2)
N(2)-C(7)-N(1)	110.9(3)	F(3)-C(14)-F(1)	108.6(7)
N(2)-C(7)-C(8)	122.7(3)	F(3)-C(14)-F(2)	104.6(7)
C(9)-C(8)-C(7)	118.9(3)	F(3)-C(14)-C(11)	115.3(6)
C(13)-C(8)-C(7)	122.6(3)	F(3A)-C(14)-C(11)	106.1(14)
C(13)-C(8-C(9)	118.3(4)		

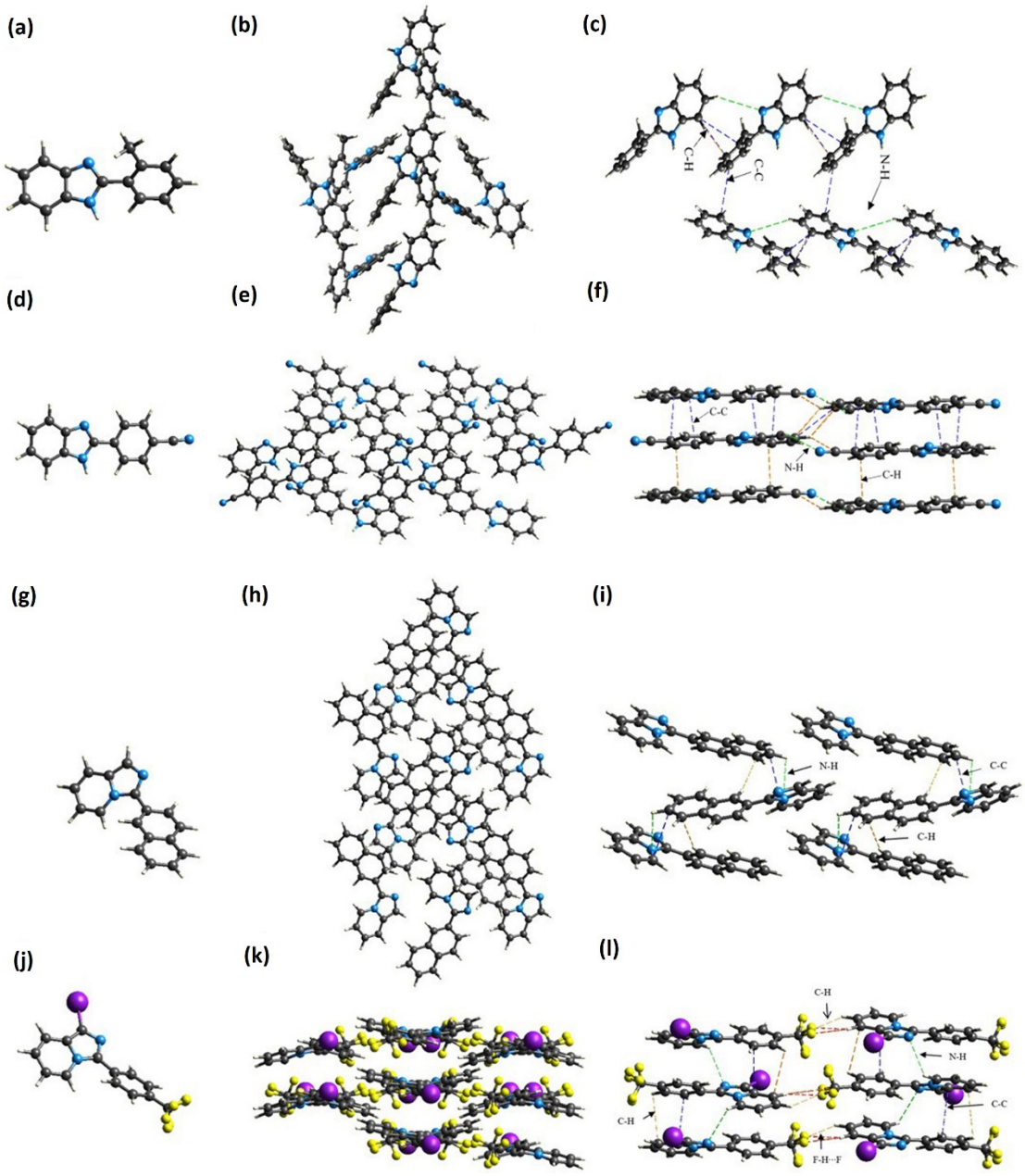


Figure S1. (a), (d), (g), (j): Single-crystal structure of **2a**, **2b**, **3a** and **3b** shown in ORTEP； (b), (e), (h), (k): Crystal packing diagram of **2a**, **2b**, **3a** and **3b**； (c), (f), (i), (l): Intermolecular interactions of **2a**, **2b**, **3a** and **3b** in the crystal lattice

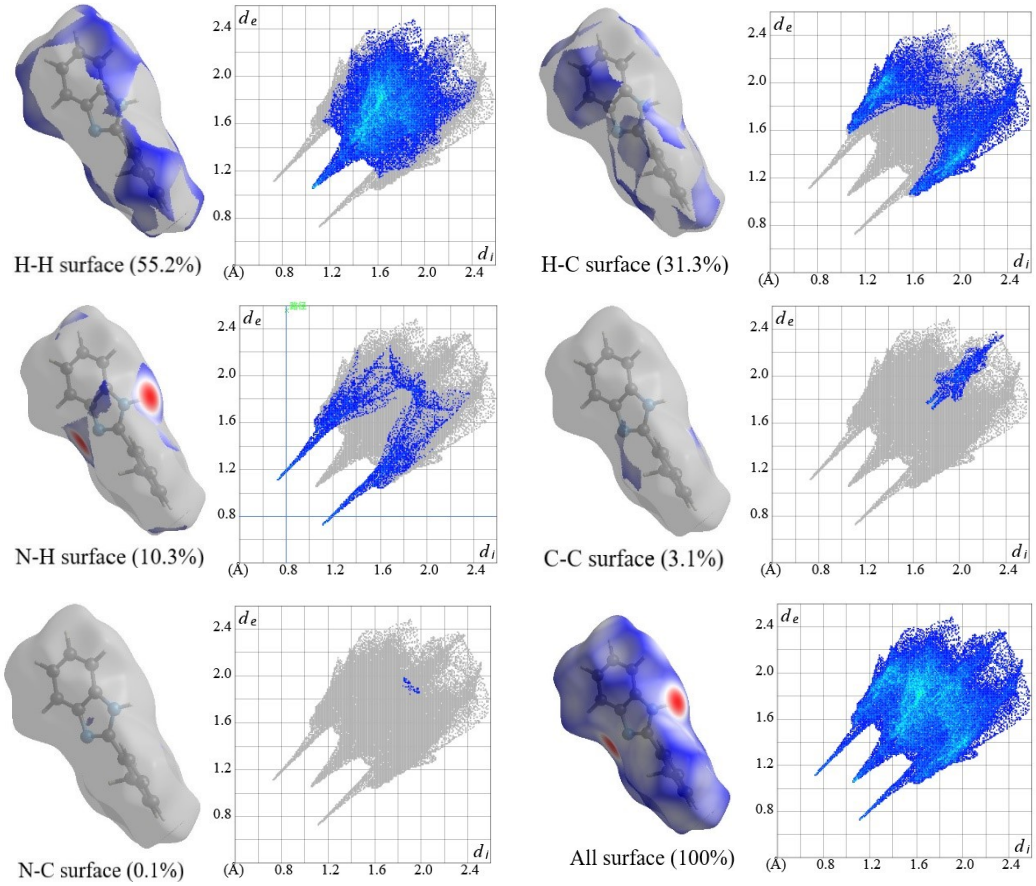


Figure S2. 2-D fingerprint plot of different contributions for the title compound **2a**.

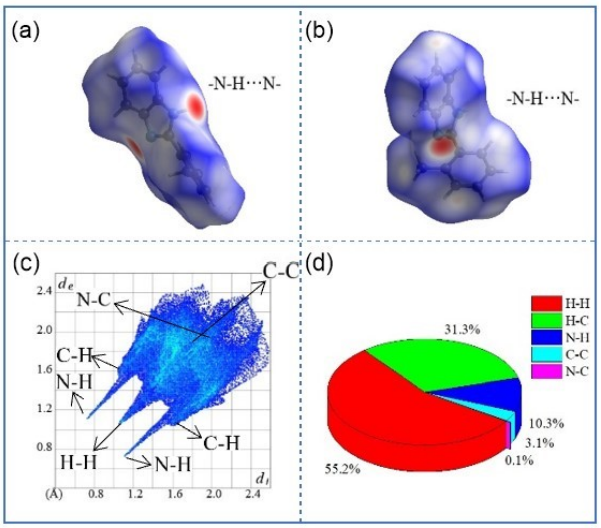


Figure S3. Hirshfeld surface (d_{norm}) of **2a** in a-axis (a) and c-axis (b) directions. (c) Fingerprint plot of **2a**. (d) The proportion of the different types of intermolecular interactions in **2a**.

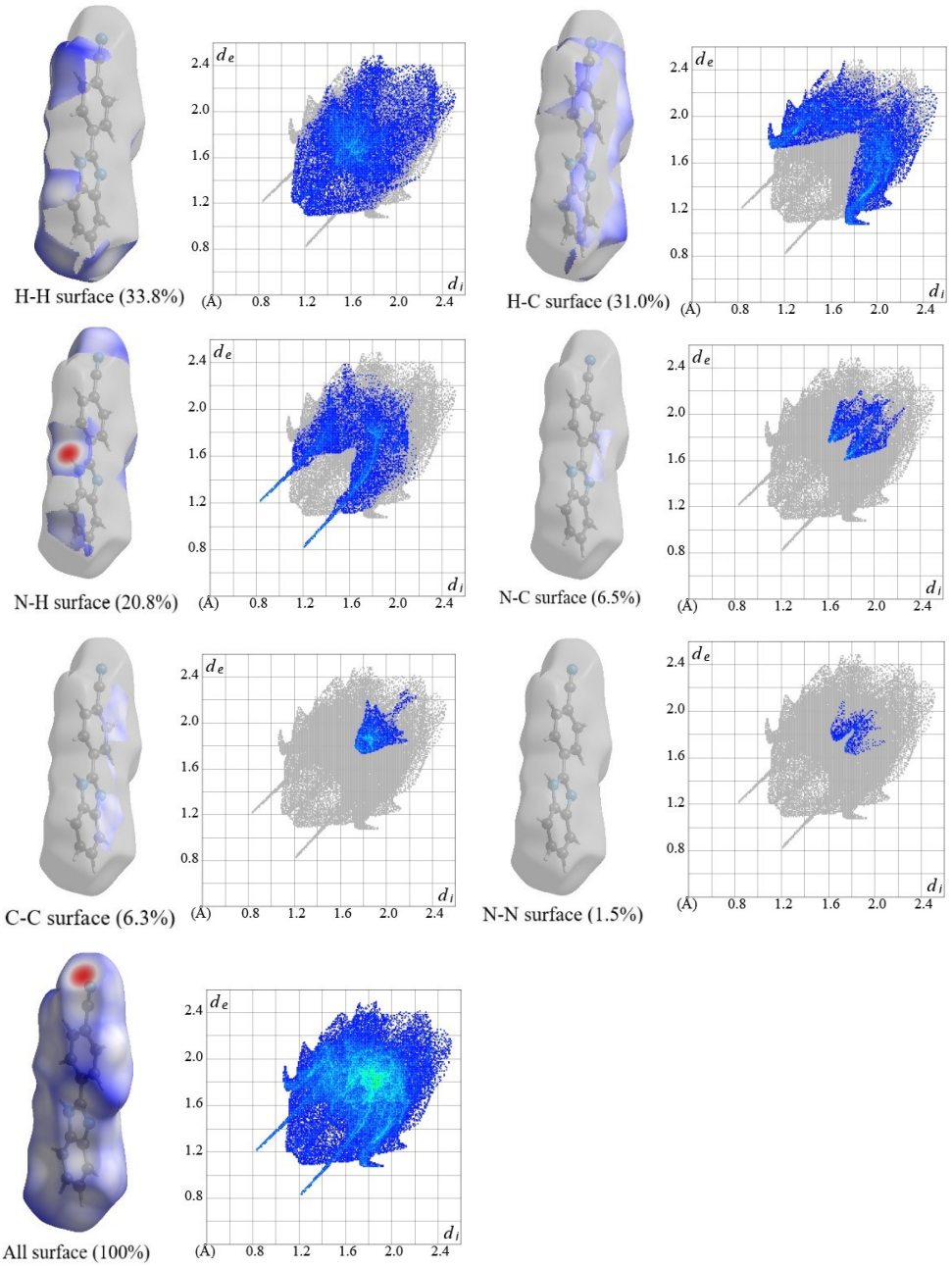


Figure S4. 2-D fingerprint plot of different contributions for the title compound **2b**.

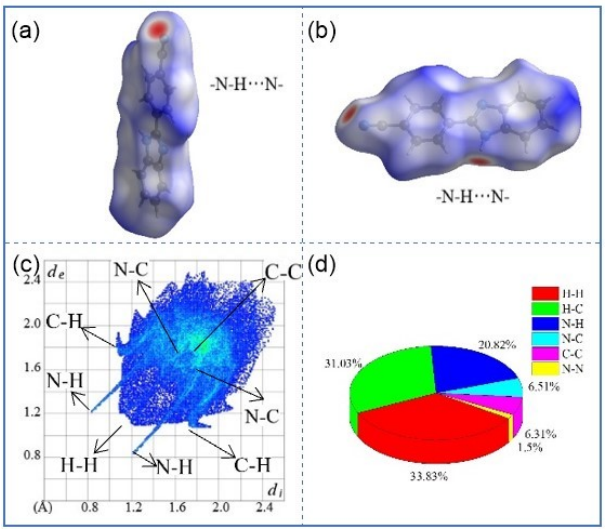


Figure S5. Hirshfeld surface (d_{norm}) of **2b** in a-axis (a) and c-axis (b) directions. (c) Fingerprint plot of **2b**. (d) The proportion of the different types of intermolecular interactions in **2b**.

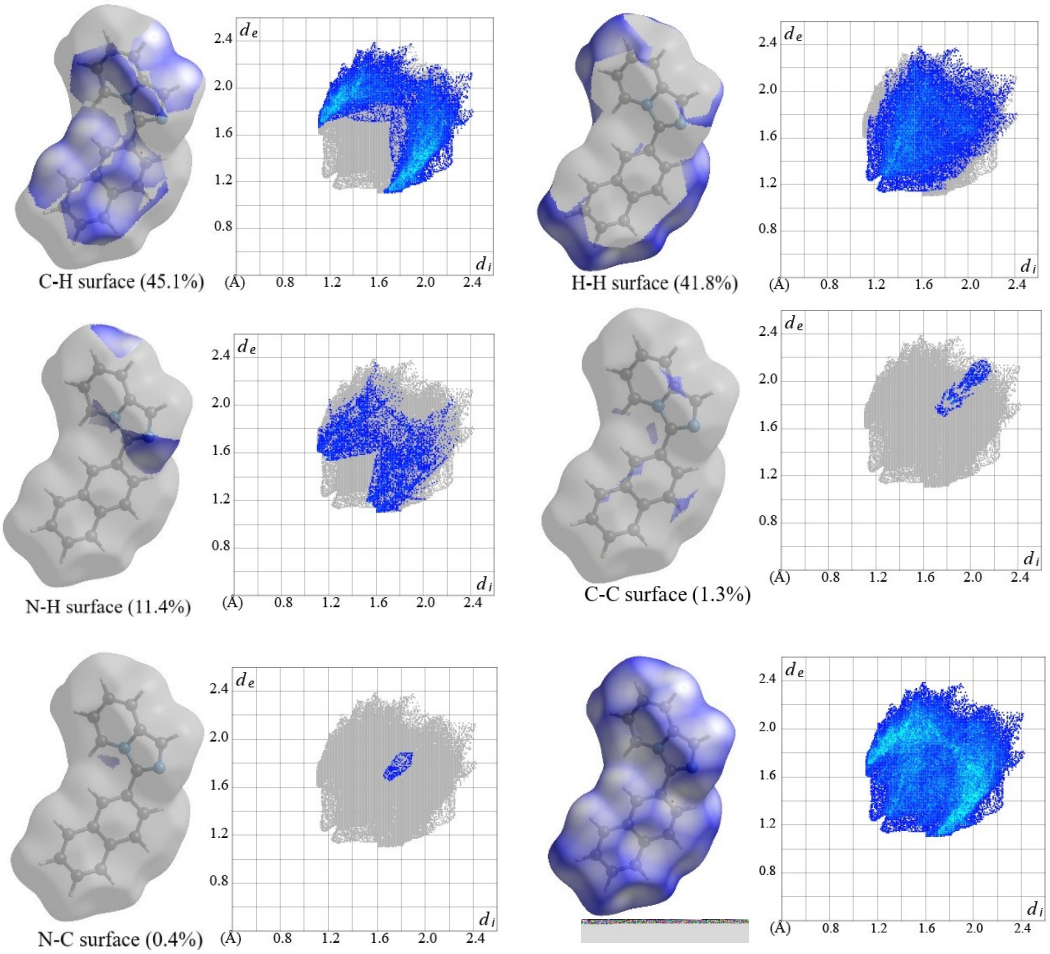


Figure S6. 2-D fingerprint plot of different contributions for the title compound **3a**.

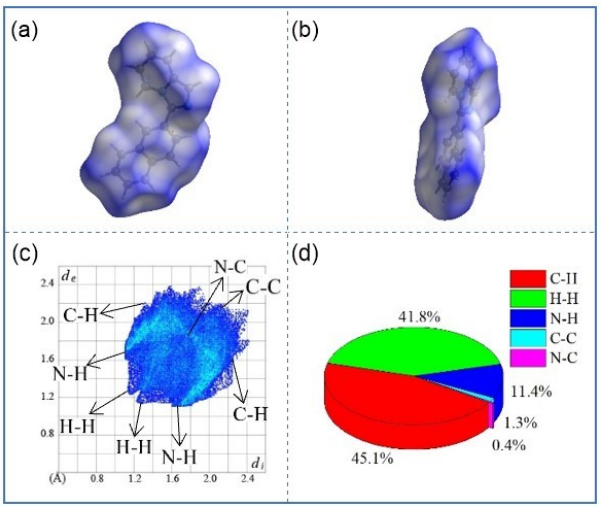


Figure S7. Hirshfeld surface (d_{norm}) of **3a** in a-axis (a) and c-axis (b) directions. (c) Fingerprint plot of **3a**. (d) The proportion of the different types of intermolecular interactions in **3a**.

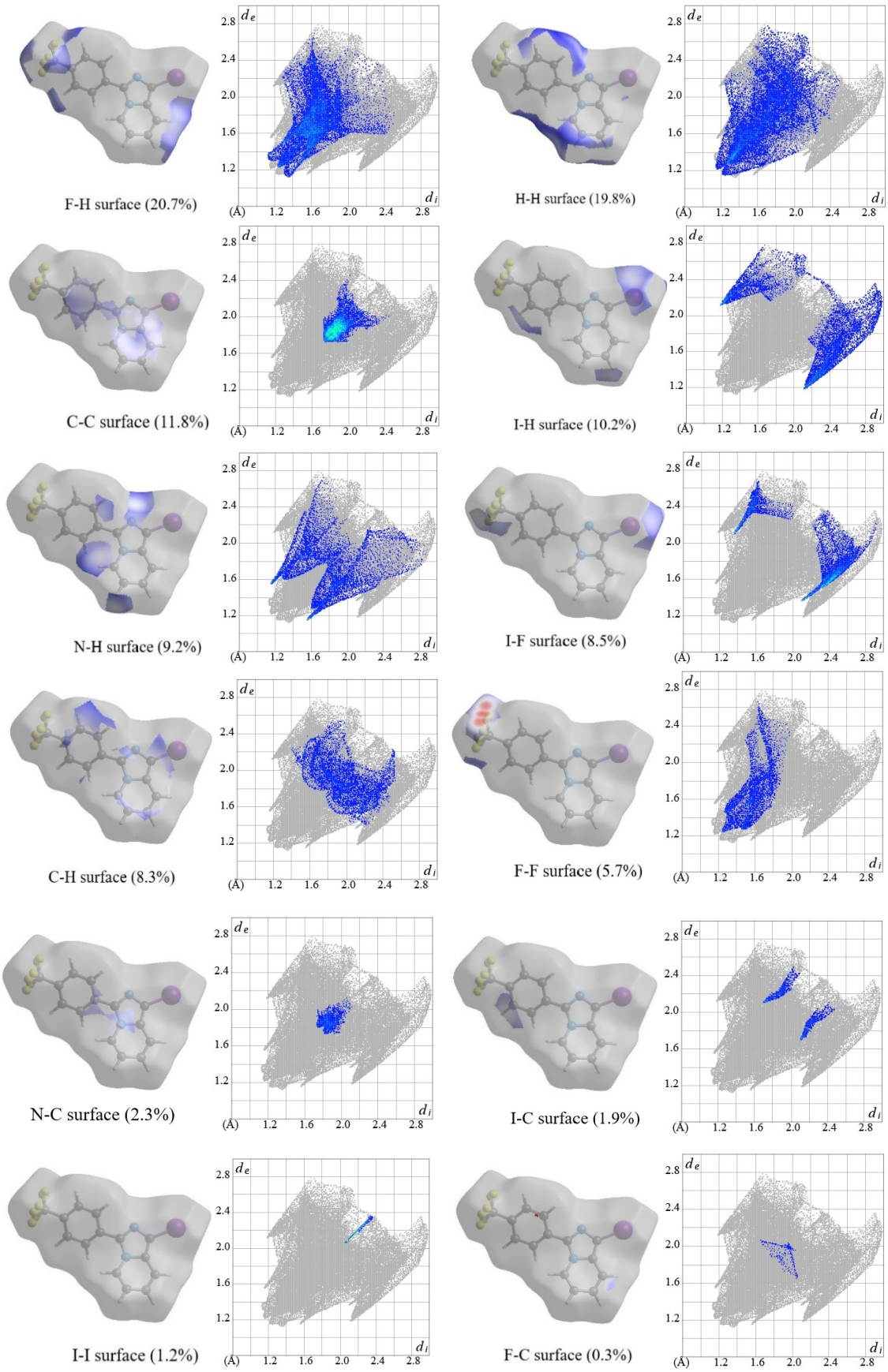


Figure S8. 2-D fingerprint plot of different contributions for the title compound **3b**.

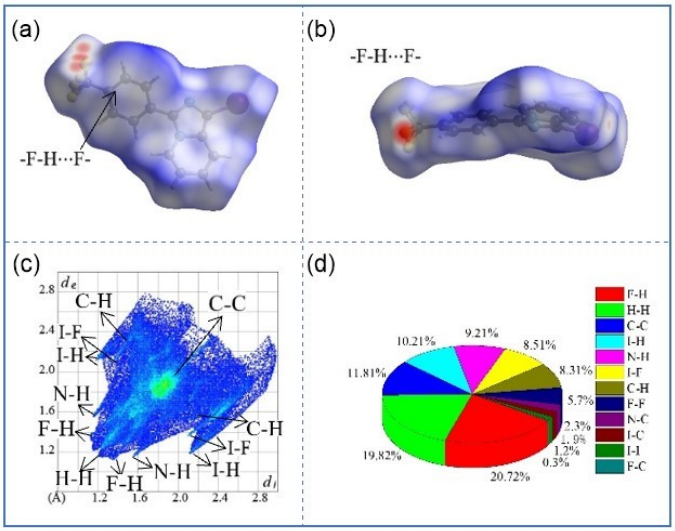


Figure S9. Hirshfeld surface (d_{norm}) of **3b** in b-axis (a) and c-axis (b) directions. (c) Fingerprint plot of **3b**. (d) The proportion of the different types of intermolecular interactions in **3b**.

3. Frontier molecular orbitals of compound 1a, 1b, 1c, 2a, 2b, 3a and **3b**

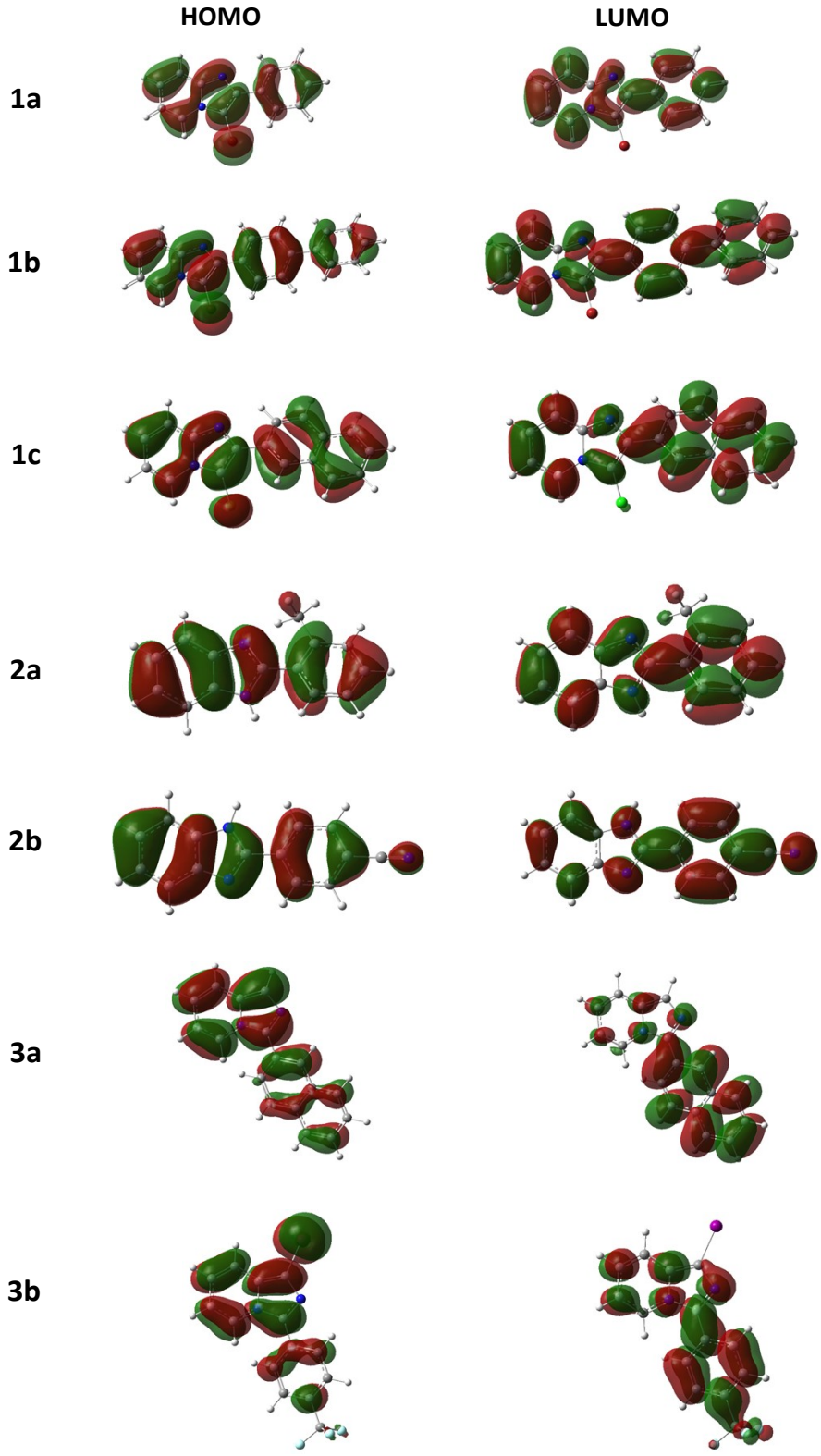


Figure S10. Frontier molecular orbitals of compounds **1a**, **1b**, **1c**, **2a**, **2b**, **3a,** and **3b** were obtained by density functional theory calculations at the B3LYP/6-31G (d) level.

4. Absorption and emission spectra of compound 1a, 1b, 1c, 2a, 2b, 3a and 3b in solution

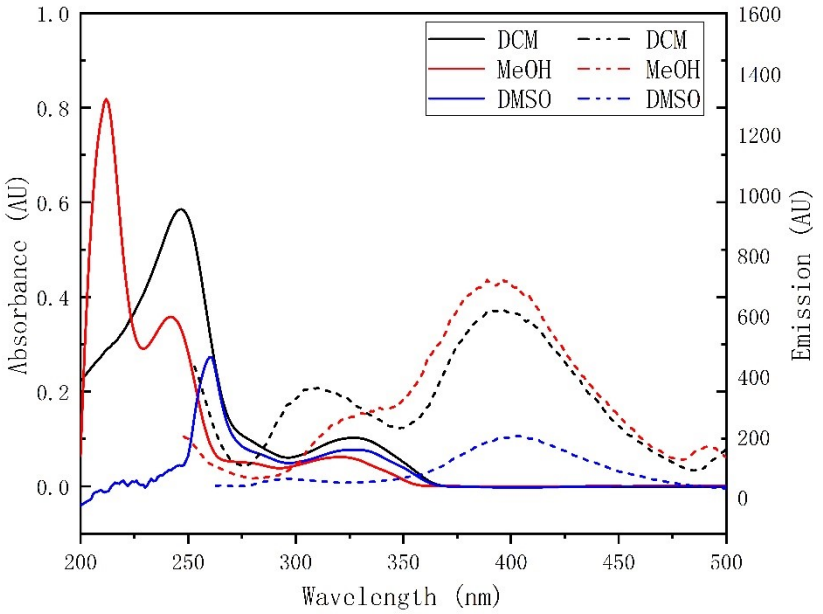


Figure S11. Absorption (solid lines, 250-500 nm) and emission (dashed lines, 250–500 nm) spectra of **1a** in three solvents of different polarity (DCM; CH_3OH; DMSO). The absorption spectra and emission spectra were taken with 1.0×10^{-5} M solutions.

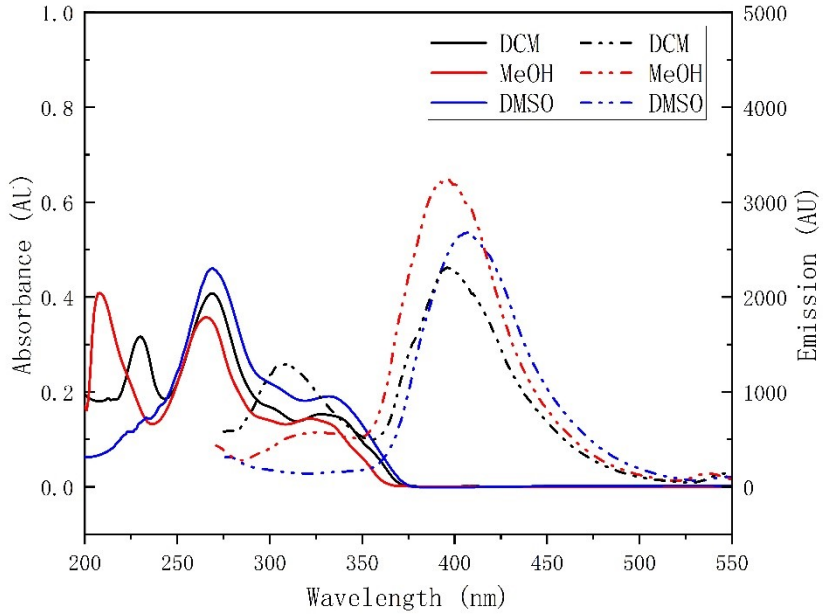


Figure S12. Absorption (solid lines, 200-500 nm) and emission (dashed lines, 275–500 nm) spectra of **1b** in three solvents of different polarity (DCM; CH_3OH; DMSO). The absorption spectra and emission spectra were taken with 1.0×10^{-5} M solutions.

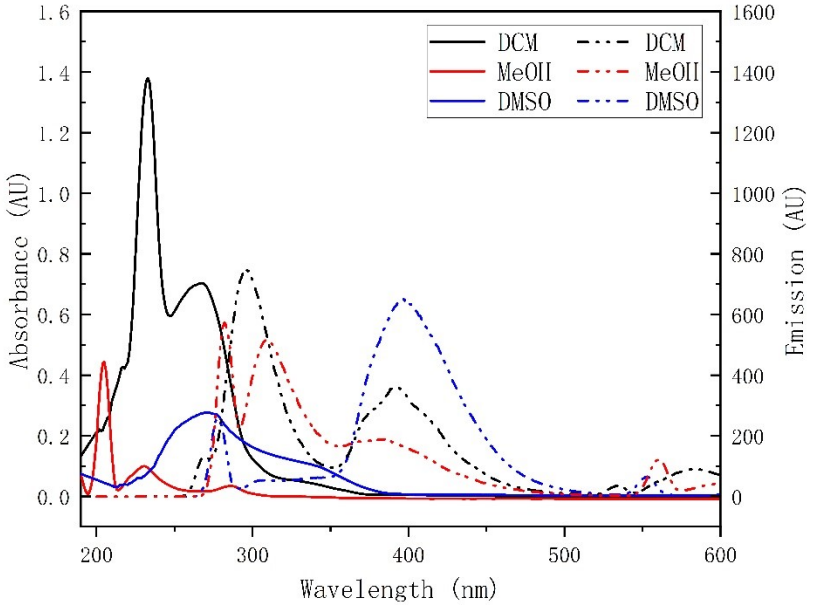


Figure S13. Absorption (solid lines, 200-500 nm) and emission (dashed lines, 250–600 nm) spectra of **1c** in three solvents of different polarity (DCM; CH_3OH; DMSO). The absorption spectra and emission spectra were taken with 1.0×10^{-5} M solutions.

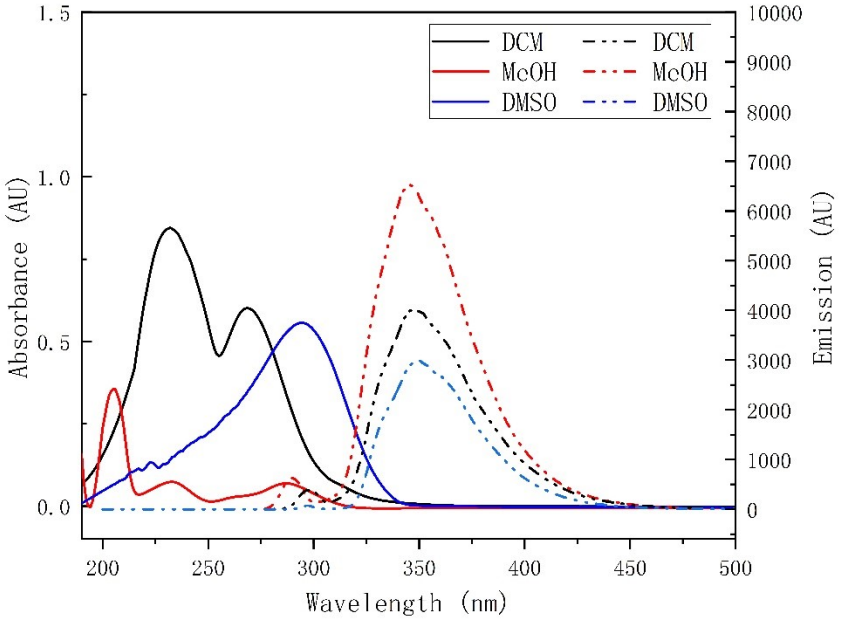


Figure S14. Absorption (solid lines, 200-500 nm) and emission (dashed lines, 275–500 nm) spectra of **2a** in three solvents of different polarity (DCM; CH_3OH; DMSO). The absorption spectra and emission spectra were taken with 1.0×10^{-5} M solutions.

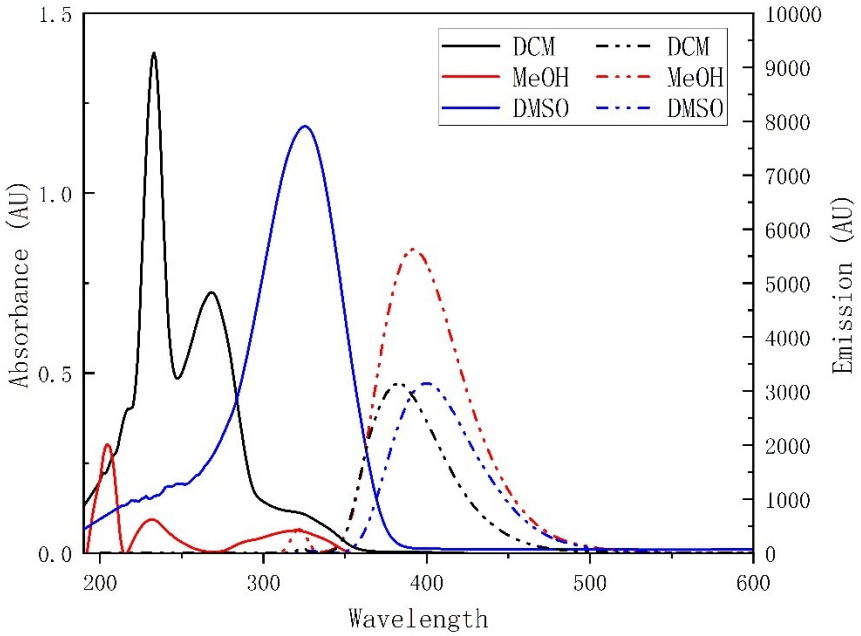


Figure S15. Absorption (solid lines, 200-500 nm) and emission (dashed lines, 300–600 nm) spectra of **2b** in three solvents of different polarity (DCM; CH_3OH; DMSO). The absorption spectra and emission spectra were taken with 1.0×10^{-5} M solutions.

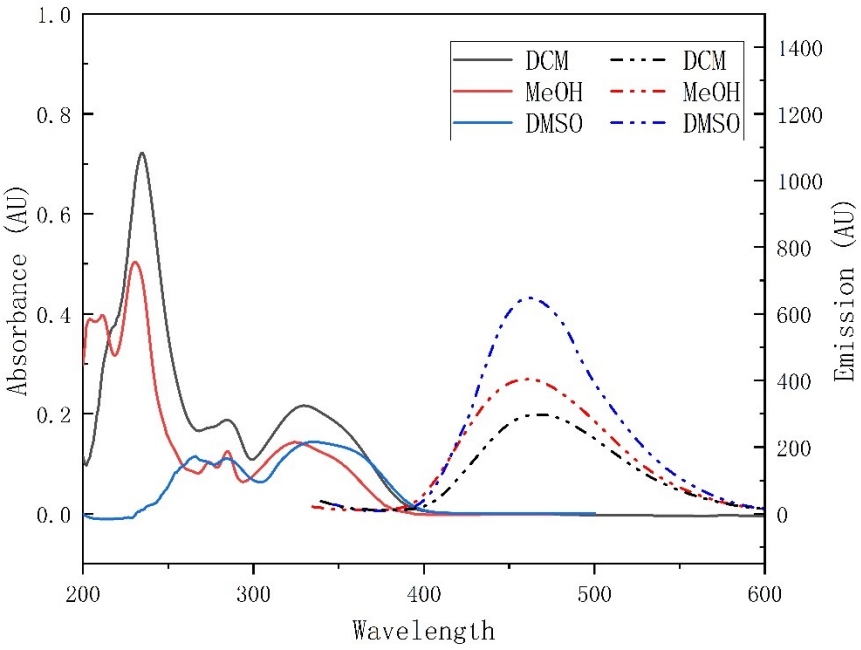


Figure S16. Absorption (solid lines, 200-500 nm) and emission (dashed lines, 325–600 nm) spectra of **3a** in three solvents of different polarity (DCM; CH_3OH; DMSO). The absorption spectra and emission spectra were taken with 1.0×10^{-5} M solutions.

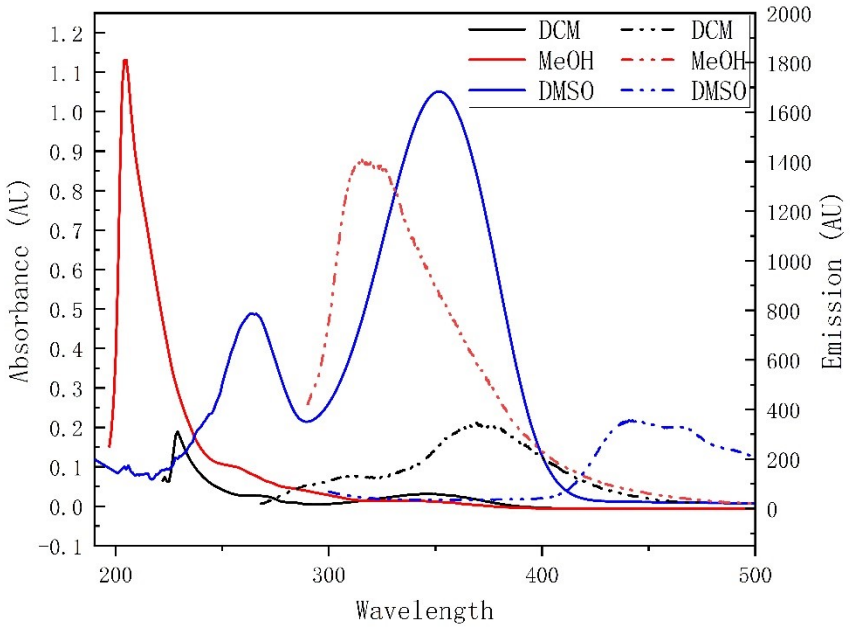


Figure S17. Absorption (solid lines, 200-500 nm) and emission (dashed lines, 275–500 nm) spectra of **3b** in three solvents of different polarity (DCM; CH_3OH; DMSO). The absorption spectra and emission spectra were taken with 1.0×10^{-5} M solutions.