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Unipolar 1-phenylimidazo[1,5-a]pyridine: A new class of ultra-bright sky blue emitters for solution-processed organic light emitting diodes

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SI1. Experimental section.

SI1.1 General information and measurements

NMR spectra (^{1}H, and ^{13}C) were recorded on an AV 400 Avance-III 400 MHz FT-NMR Spectrometer (Bruker Biospin International, Switzerland) with tetramethylsilane (TMS) as standard reference and Mass spectra of all the synthesized fluorophores were recorded on

High Resolution Mass Spectrometer (HRMS) Waters, USA, XEVO G2-XS QTOF model. The FT-IR spectra were recorded on a Perkin–Elmer RX-I FTIR spectrophotometer. Themogravimetric analysis (TGA) was performed using TA Instrument TGAQ50 thermal analysis system. UV-Vis absorption was measured using UV-vis spectrophotometer (Shimadzu Corporation, japan/UV-2450 pekin Elmer, USA/Lamda 25) and photoluminescence (PL) spectra were recorded using an Edinburgh instrument FLS980 spectrofluorometer. The absolute PL Quantum yields (PLQY) were measured using an Edinburgh instrument spectrofluorometer, integrating sphere SC-30 model. The quantum yield of the fluorophores is calculated by using equation (1).

$$\Phi = \frac{L_0(\lambda) - L_i(\lambda)}{L_0(\lambda)} \quad (1)$$

$$\eta = \frac{E_i(\lambda) - (1 - \Phi)E_0(\lambda)}{E_0(\lambda)\Phi}$$

Where, $L_0(\lambda)$ is the integrated excitation profile (sample is directly excited by the incident beam) and $L_i(\lambda)$ are the integrated excitation profile attained from the empty integrated sphere. $E_0(\lambda)$ is the integrated luminescence of solid caused by direct excitation and Ei(λ) is indirect illumination from the sphere, respectively. Photoluminescence lifetime of the dyes was measured at 298 K with an Edinburgh Instrument FLS 980 luminescence spectrometer based on the time correlated single photon counting technology for all the dyes. Cyclic voltammetry (CV) of the fluorophores were carried out by using AUTOLAB 302 Modular Potentiostat electrochemical analyzer at 298 ± 1 K. The tests were carried out in dimethylformamide (DMF) containing 0.1 M tetrabutylammonium perchlorate (Bu_4NClO_4) as a supporting electrolyte, and the scan rate were maintained at 100 mVs^{-1} with three conventional electrode configurations viz, a glassy carbon working electrode, a platinum

plate auxiliary electrode, and an Ag/AgCl reference electrode. The single crystal analysis was carried out by using Rigaku oxford diffraction (XtaLAB Pro II AFC12 (RINC): Kα single diffractometer) using Mo k α as radiation source.

SI1.2 Computational details

The optimized geometries and relevant energies of the ImPy derivatives were obtained by means of density functional theory (DFT) calculations using the hybrid B3LYP functional and 6-311G (d, p) basis set. At the same time, the absorption spectrum of ImPy derivatives were carried out by time-dependent density functional theory (TD-DFT) with B3LYP functional and the basis set 6-311G (d, p) based on the optimized S0 state geometry in the gas phase. All geometries were confirmed to be minima by additional vibrational frequency calculations. The singlet and lowest triplet energies were evaluated via the Δ self-consistent field (ΔSCF) method based on optimized geometries. All the DFT and TD-DFT calculations were conducted using the Gaussian 09 software package and Gauss View suite of programs for the studied system.[1]

SI1.3 Device fabrication and measurements

ImPy based solution-processed sky-blue OLED were fabricated on a precleaned 150 nm patterned ITO substrate, cleaning process involve washing with detergent, sonication in acetone and isopropyl alcohol for 60 minutes then exposed under UV light for 15 minutes. A 30 nm layer of 3,4-ethylenedioxythiophene-poly(styrenesulfonate) (PEDOT: PSS) was spin-coated at 4500 rpm for 20 s then heat-treated at 140 °C for 20 min as hole injection layer. Further, CBP (4,4′-bis(N-carbazolyl)-1,1′-biphenyl) as a host and X wt % of ImPy based material were used as blue emitter dissolved in (THF) and an emissive layer of 20 nm was spin-coated at 2500 rpm for 20 s. All the spin coating was performed in a glovebox under in the nitrogen atmosphere. A 30 nm of an electron transporting layer TPBi (2,2′,2″-(1,3,5-benzinetriyl)-tris(1-phenyl-1-H-benzimidazole)), 1 nm of LiF (lithium fluoride) as an electron

injection layer, an anode of 150 nm aluminium were deposited by thermal evaporation under high vacuum (6×10^{-6} Torr).

SI2. NMR (^{1}H and ^{13}C) spectra of ImPy-derivatives.

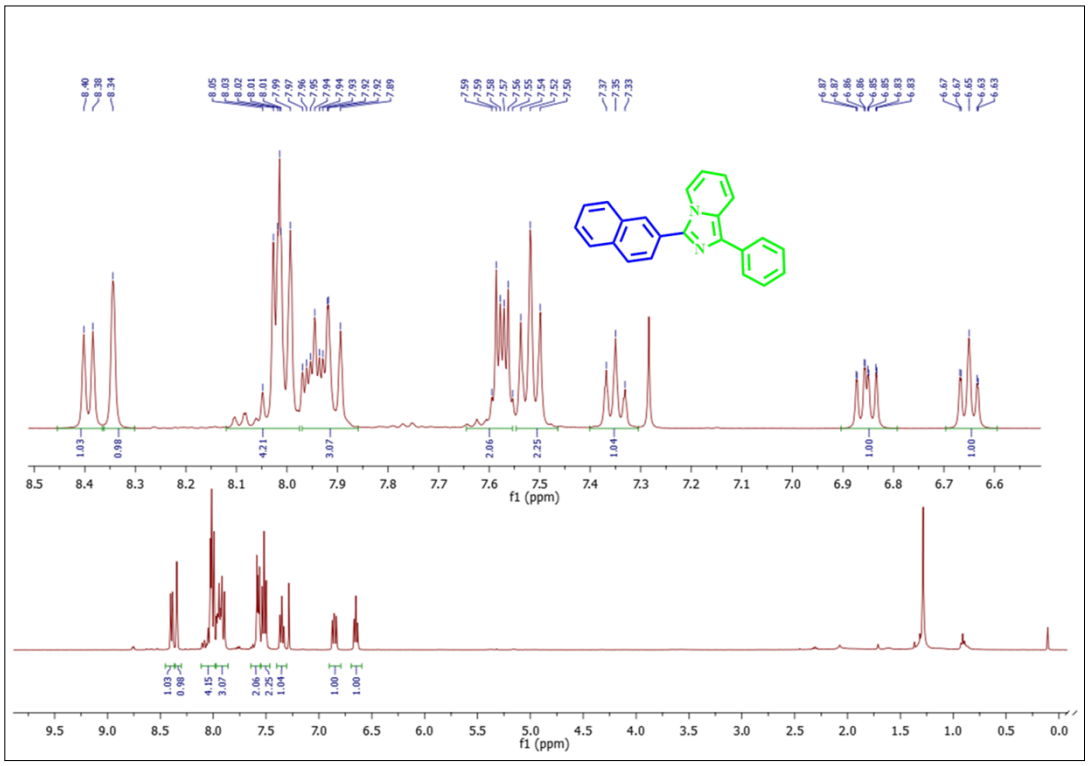


Fig. S1. ^{1}H NMR spectra of ImPy-1.

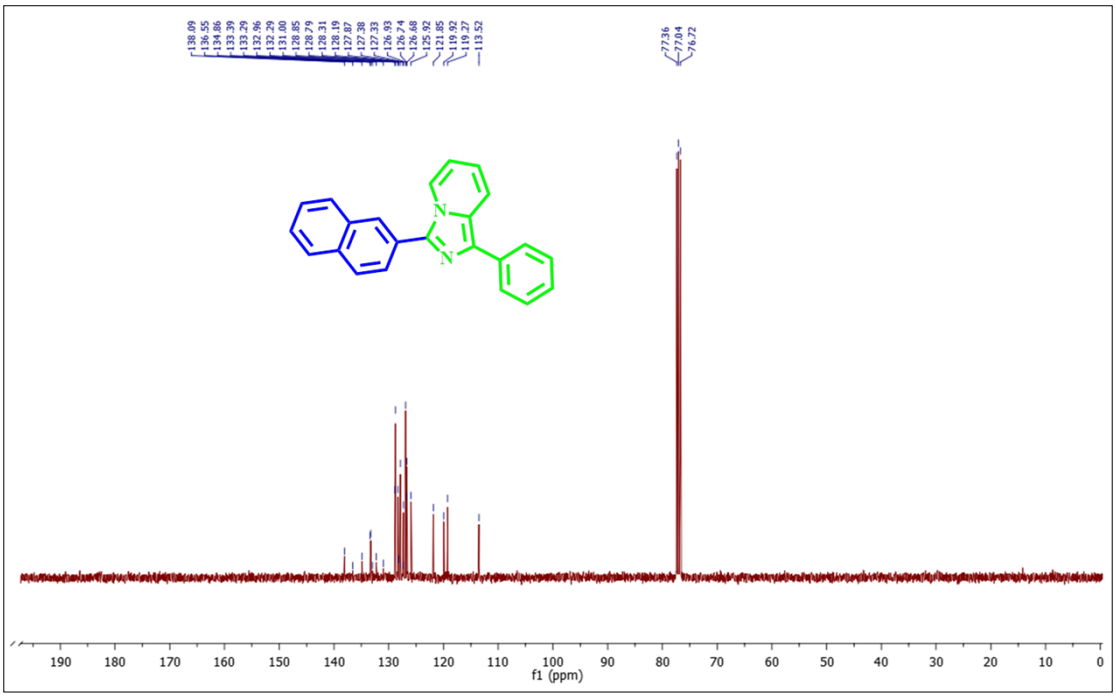


Fig. S2. ^{13}C NMR spectra of ImPy-1.

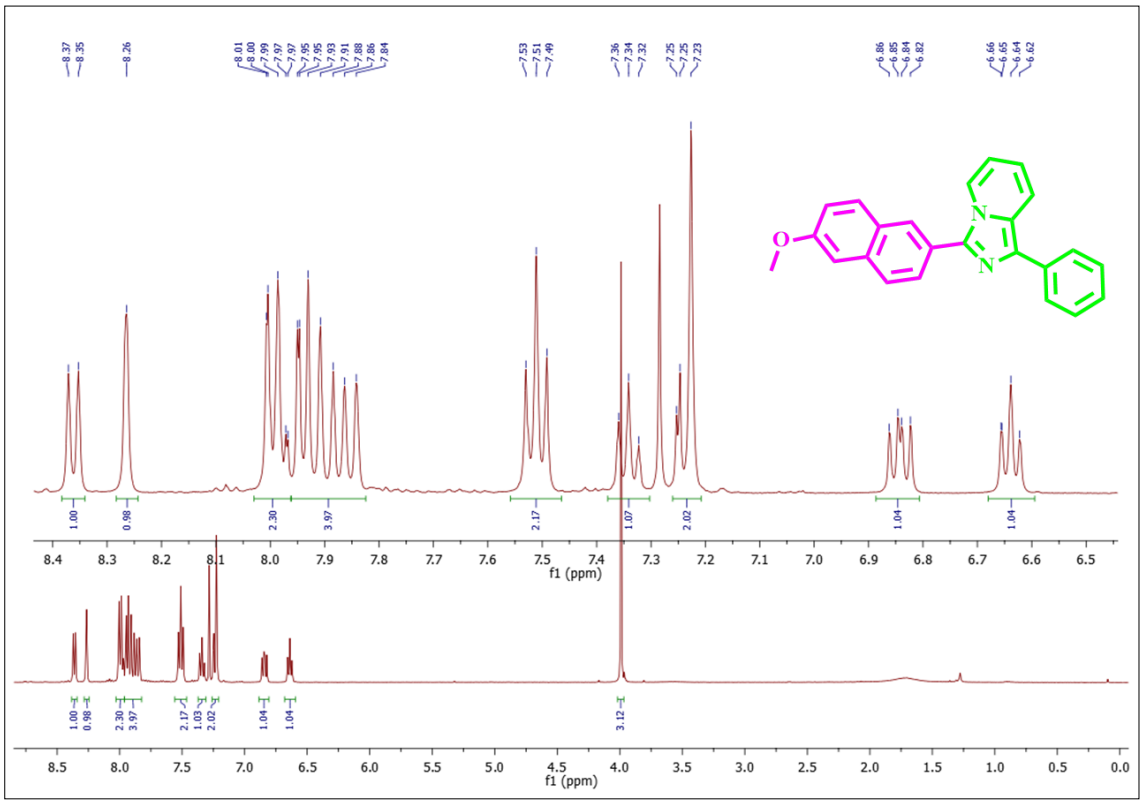


Fig. S3. ^{1}H NMR spectra of ImPy-2.

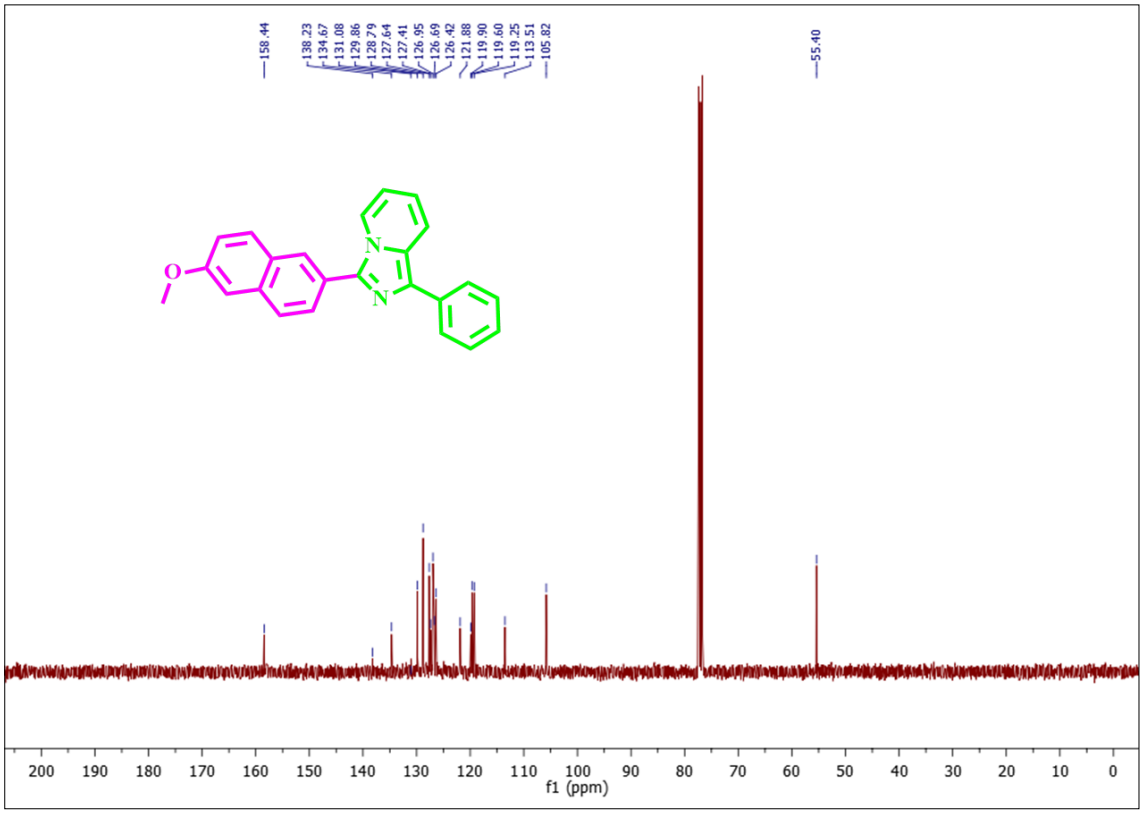


Fig. S4. ^{13}C NMR spectra of ImPy-2.

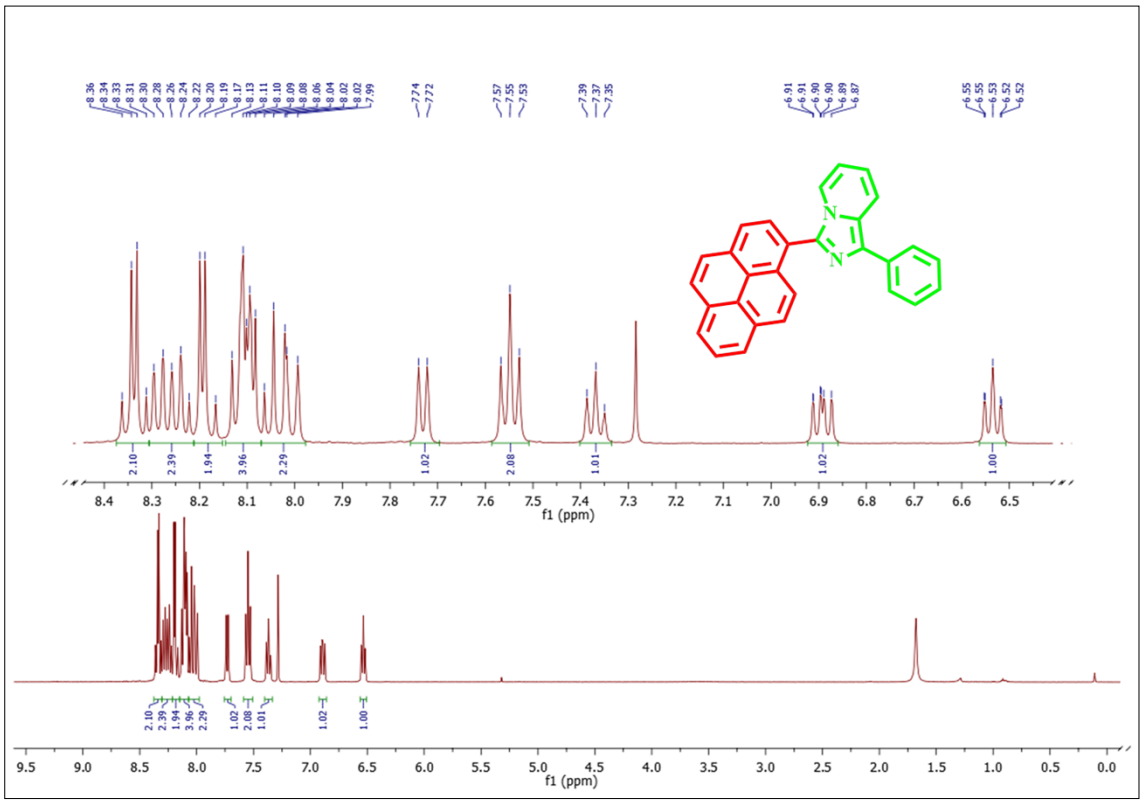


Fig. S5. ^{1}H NMR spectra of ImPy-3.

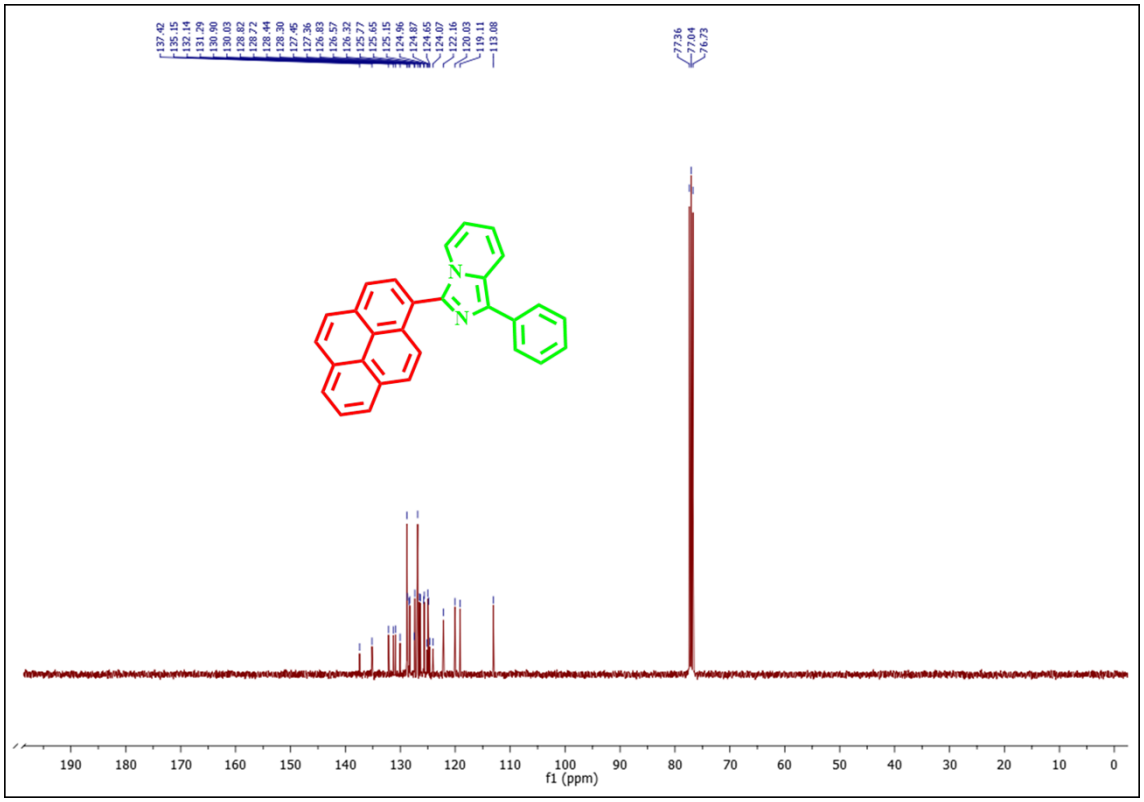


Fig. S6. ^{13}C NMR spectra of ImPy-3.

SI3. Mass spectra of the molecules.

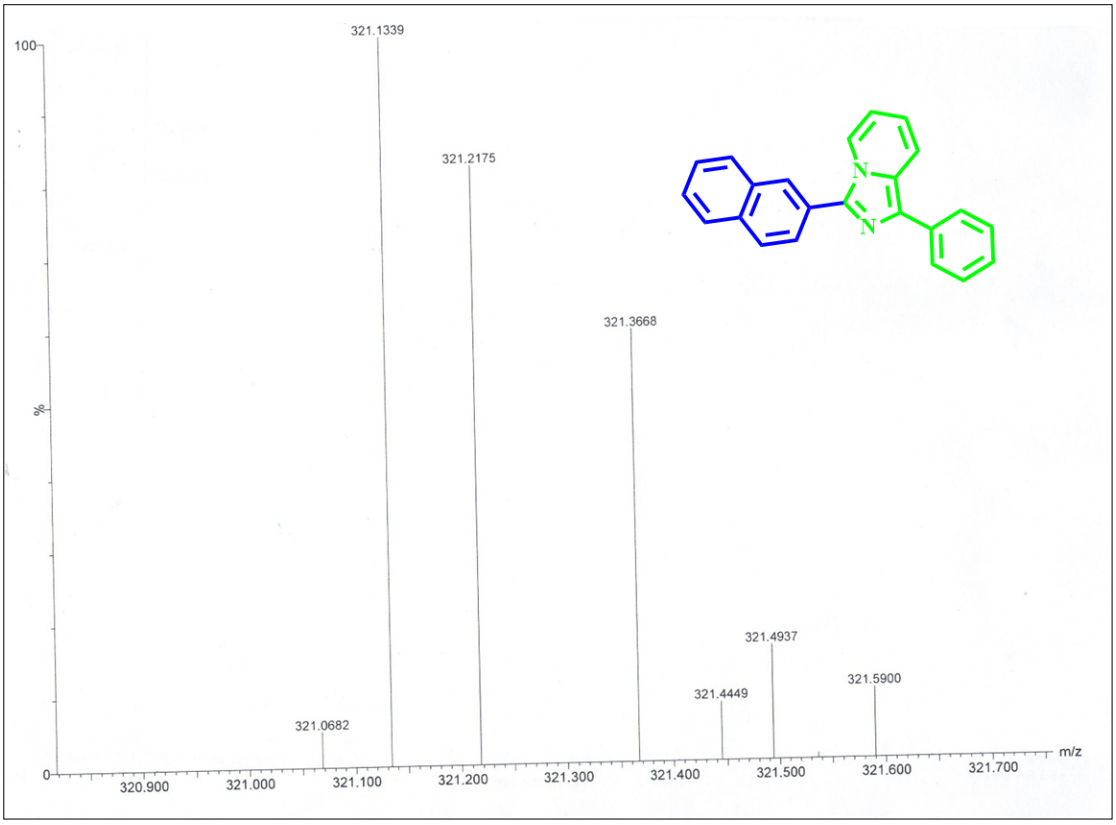


Fig. S7. Mass spectra of ImPy-1.

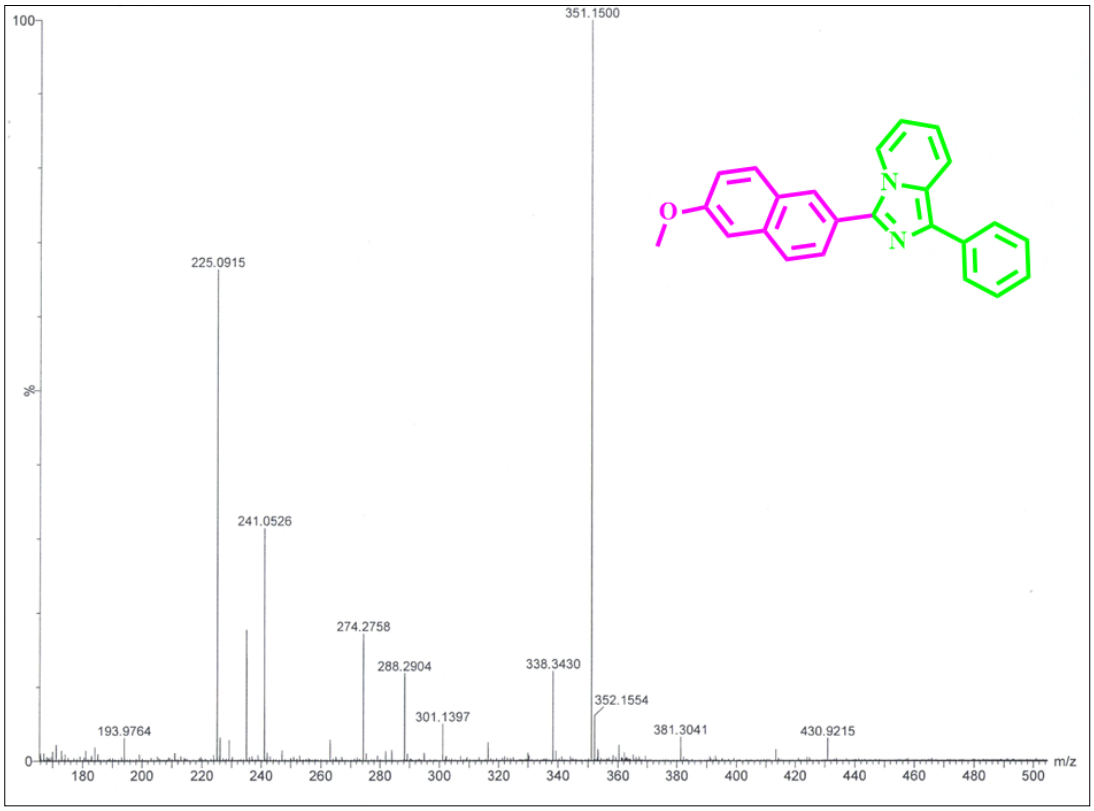


Fig. S8. Mass spectra of ImPy-2.

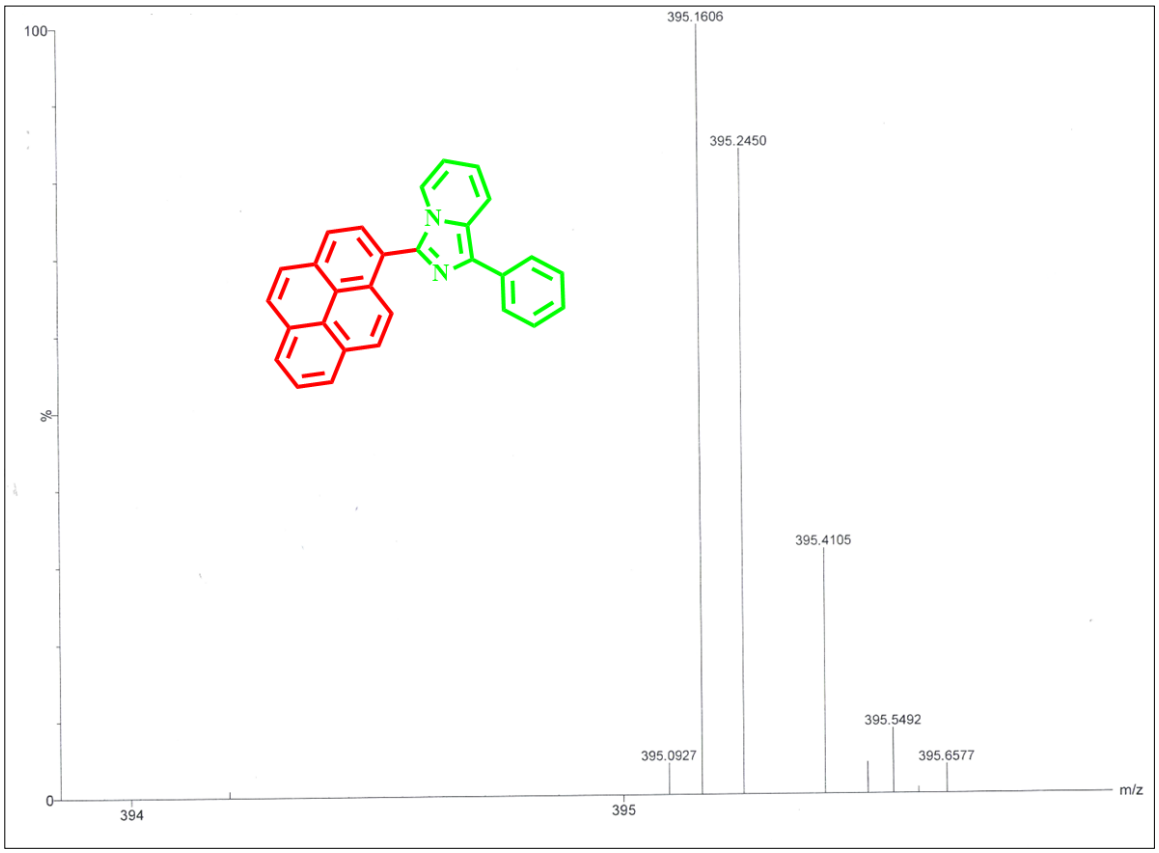


Fig. S9. Mass spectra of ImPy-3.

SI4. Single crystal analysis of ImPy-1 and ImPy-3.

Table ST1. Bond Lengths for ImPy-1.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
N(001)	C(008)	1.3781(15)		C(00P)	C(00W)	1.3534(17)
N(001)	C(00L)	1.3890(15)		C(00P)	H(00P)	0.9300
N(001)	C(005)	1.4027(14)		C(00Q)	C(010)	1.3486(19)
N(002)	C(00C)	1.3795(16)		C(00Q)	H(00Q)	0.9300
N(002)	C(00U)	1.3870(16)		C(00R)	C(00X)	1.3814(16)
N(002)	C(009)	1.4038(14)		C(00R)	H(00R)	0.9300
N(003)	C(008)	1.3269(15)		C(00S)	C(012)	1.3504(18)
N(003)	C(006)	1.3648(14)		C(00S)	H(00S)	0.9300
N(004)	C(00C)	1.3252(14)		C(00T)	C(019)	1.3766(18)
N(004)	C(00G)	1.3679(15)		C(00T)	H(00T)	0.9300
C(005)	C(006)	1.3891(18)		C(00U)	C(017)	1.3410(19)
C(005)	C(00Q)	1.4103(17)		C(00U)	H(00U)	0.9300
C(006)	C(00I)	1.4694(16)		C(00V)	C(018)	1.360(2)
C(007)	C(00H)	1.3788(16)		C(00V)	H(00V)	0.9300
C(007)	C(00P)	1.4175(18)		C(00W)	H(00W)	0.9300
C(007)	C(00C)	1.4629(16)		C(00X)	C(014)	1.3850(19)
C(008)	C(00D)	1.4637(16)		C(00X)	H(00X)	0.9300

C(009)	C(00G)	1.3860(17)		C(00Y)	C(010)	1.4178(18)
C(009)	C(00S)	1.4130(17)		C(00Y)	H(00Y)	0.9300
C(00A)	C(00N)	1.4129(17)		C(00Z)	C(01C)	1.3760(18)
C(00A)	C(00V)	1.4148(16)		C(00Z)	H(00Z)	0.9300
C(00A)	C(00B)	1.4214(18)		C(010)	H(010)	0.9300
C(00B)	C(00E)	1.4138(16)		C(011)	C(01B)	1.3601(19)
C(00B)	C(013)	1.4171(18)		C(011)	H(011)	0.9300
C(00D)	C(00E)	1.3802(17)		C(012)	C(017)	1.4138(19)
C(00D)	C(00M)	1.4219(17)		C(012)	H(012)	0.9300
C(00E)	H(00E)	0.9300		C(013)	C(01A)	1.3652(17)
C(00F)	C(00H)	1.4116(16)		C(013)	H(013)	0.9300
C(00F)	C(00J)	1.4138(18)		C(014)	C(015)	1.379(2)
C(00F)	C(011)	1.4143(16)		C(014)	H(014)	0.9300
C(00G)	C(00K)	1.4666(16)		C(015)	H(015)	0.9300
C(00H)	H(00H)	0.9300		C(016)	C(01E)	1.363(2)
C(00I)	C(00T)	1.3902(18)		C(016)	H(016)	0.9300
C(00I)	C(00Z)	1.3919(17)		C(017)	H(017)	0.9300
C(00J)	C(016)	1.4124(17)		C(018)	C(01A)	1.402(2)
C(00J)	C(00W)	1.4164(18)		C(018)	H(018)	0.9300
C(00K)	C(00R)	1.3945(18)		C(019)	C(01D)	1.379(2)
C(00K)	C(00O)	1.3999(17)		C(019)	H(019)	0.9300
C(00L)	C(00Y)	1.3410(17)		C(01A)	H(01A)	0.9300
C(00L)	H(00L)	0.9300		C(01B)	C(01E)	1.394(2)
C(00M)	C(00N)	1.3581(16)		C(01B)	H(01B)	0.9300
C(00M)	H(00M)	0.9300		C(01C)	C(01D)	1.372(2)
C(00N)	H(00N)	0.9300		C(01C)	H(01C)	0.9300
C(00O)	C(015)	1.3781(17)		C(01D)	H(01D)	0.9300
C(00O)	H(00O)	0.9300		C(01E)	H(01E)	0.9300

Table ST2. Bond angles for ImPy-1.

Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
C(008)	N(001)	C(00L	132.00(10)		C(005)	C(00Q)	H(00Q)	119.9
C(008)	N(001)	C(005)	106.98(10)		C(00X)	C(00R)	C(00K)	120.82(12)
C(00L)	N(001)	C(005)	120.92(10)		C(00X)	C(00R)	H(00R)	119.6
C(00C)	N(002)	C(00U)	132.26(10)		C(00K)	C(00R)	H(00R)	119.6
C(00C)	N(002)	C(009)	107.01(9)		C(012)	C(00S)	C(009)	120.10(12)
C(00U)	N(002)	C(009)	120.64(11)		C(012)	C(00S)	H(00S)	119.9
C(008)	N(003)	C(006)	107.36(10)		C(009)	C(00S)	H(00S)	119.9
C(00C)	N(004)	C(00G)	107.48(10)		C(019)	C(00T)	C(00I)	120.57(13)
C(006)	C(005)	N(001)	105.16(10)		C(019)	C(00T)	H(00T)	119.7
C(006)	C(005)	C(00Q)	136.77(11)		C(00I)	C(00T)	H(00T)	119.7
N(001)	C(005)	C(00Q)	118.00(11)		C(017)	C(00U)	N(002)	119.48(12)
N(003)	C(006)	C(005)	109.95(10)		C(017)	C(00U)	H(00U)	120.3
N(003)	C(006)	C(00I)	122.81(11)		N(002)	C(00U)	H(00U)	120.3
C(005)	C(006)	C(00I)	127.24(10)		C(018)	C(00V)	C(00A)	120.97(13)
C(00H)	C(007)	C(00P)	118.05(11)		C(018)	C(00V)	H(00V)	119.5

C(00H)	C(007)	C(00C)	123.97(12)		C(00A)	C(00V)	H(00V)	119.5
C(00P)	C(007)	C(00C)	117.96(10)		C(00P)	C(00W)	C(00J)	121.61(13)
N(003)	C(008)	N(001)	110.52(10)		C(00P)	C(00W)	H(00W)	119.2
N(003)	C(008)	C(00D)	123.59(11)		C(00J)	C(00W)	H(00W)	119.2
N(001)	C(008)	C(00D)	125.85(11)		C(00R)	C(00X)	C(014)	120.30(13)
C(00G)	C(009)	N(002)	105.23(10)		C(00R)	C(00X)	H(00X)	119.8
C(00G)	C(009)	C(00S)	136.37(12)		C(014)	C(00X)	H(00X)	119.8
N(002)	C(009)	C(00S)	118.37(11)		C(00L)	C(00Y)	C(010)	120.80(13)
C(00N)	C(00A)	C(00V)	122.96(12)		C(00L)	C(00Y)	H(00Y)	119.6
C(00N)	C(00A)	C(00B)	118.13(11)		C(010)	C(00Y)	H(00Y)	119.6
C(00V)	C(00A)	C(00B)	118.91(12)		C(01C)	C(00Z)	C(00I)	121.37(14)
C(00E)	C(00B)	C(013)	122.26(12)		C(01C)	C(00Z)	H(00Z)	119.3
C(00E)	C(00B)	C(00A)	119.30(11)		C(00I)	C(00Z)	H(00Z)	119.3
C(013)	C(00B)	C(00A)	118.44(11)		C(00Q)	C(010)	C(00Y)	120.17(12)
N(004)	C(00C)	N(002)	110.40(10)		C(00Q)	C(010)	H(010)	119.9
N(004)	C(00C)	C(007)	124.03(12)		C(00Y)	C(010)	H(010)	119.9
N(002)	C(00C)	C(007)	125.56(11)		C(01B)	C(011)	C(00F)	120.95(14)
C(00E)	C(00D)	C(00M)	118.41(11)		C(01B)	C(011)	H(011)	119.5
C(00E)	C(00D)	C(008)	124.16(12)		C(00F)	C(011)	H(011)	119.5
C(00M)	C(00D)	C(008)	117.37(11)		C(00S)	C(012)	C(017)	119.88(13)
C(00D)	C(00E)	C(00B)	121.51(12)		C(00S)	C(012)	H(012)	120.1
C(00D)	C(00E)	H(00E)	119.2		C(017)	C(012)	H(012)	120.1
C(00B)	C(00E)	H(00E)	119.2		C(01A)	C(013)	C(00B)	120.91(13)
C(00H)	C(00F)	C(00J)	119.14(11)		C(01A)	C(013)	H(013)	119.5
C(00H)	C(00F)	C(011)	122.34(12)		C(00B)	C(013)	H(013)	119.5
C(00J)	C(00F)	C(011)	118.51(11)		C(015)	C(014)	C(00X)	119.62(12)
N(004)	C(00G)	C(009)	109.88(10)		C(015)	C(014)	H(014)	120.2
N(004)	C(00G)	C(00K)	121.23(11)		C(00X)	C(014)	H(014)	120.2
C(009)	C(00G)	C(00K)	128.89(11)		C(00O)	C(015)	C(014)	120.30(13)
C(007)	C(00H)	C(00F)	121.90(12)		C(00O)	C(015)	H(015)	119.8
C(007)	C(00H)	H(00H)	119.0		C(014)	C(015)	H(015)	119.8
C(00F)	C(00H)	H(00H)	119.0		C(01E)	C(016)	C(00J)	120.42(15)
C(00T)	C(00I)	C(00Z)	117.72(11)		C(01E)	C(016)	H(016)	119.8
C(00T)	C(00I)	C(006)	121.86(11)		C(00J)	C(016)	H(016)	119.8
C(00Z)	C(00I)	C(006)	120.42(12)		C(00U)	C(017)	C(012)	121.35(13)
C(016)	C(00J)	C(00F)	119.12(12)		C(00U)	C(017)	H(017)	119.3
C(016)	C(00J)	C(00W)	122.83(13)		C(012)	C(017)	H(017)	119.3
C(00F)	C(00J)	C(00W)	118.05(11)		C(00V)	C(018)	C(01A)	120.34(13)
C(00R)	C(00K)	C(00O)	117.96(11)		C(00V)	C(018)	H(018)	119.8
C(00R)	C(00K)	C(00G)	120.37(11)		C(01A)	C(018)	H(018)	119.8
C(00O)	C(00K)	C(00G)	121.62(12)		C(00T)	C(019)	C(01D)	120.82(15)
C(00Y)	C(00L)	N(001)	119.49(12)		C(00T)	C(019)	H(019)	119.6
C(00Y)	C(00L)	H(00L)	120.3		C(01D)	C(019)	H(019)	119.6
N(001)	C(00L)	H(00L)	120.3		C(013)	C(01A)	C(018)	120.41(13)
C(00N)	C(00M)	C(00D)	121.04(12)		C(013)	C(01A)	H(01A)	119.8
C(00N)	C(00M)	H(00M)	119.5		C(018)	C(01A)	H(01A)	119.8
C(00D)	C(00M)	H(00M)	119.5		C(011)	C(01B)	C(01E)	120.30(13)

C(00M)	C(00N)	C(00A)	121.59(12)		C(011)	C(01B)	H(01B)	119.8
C(00M)	C(00N)	H(00N)	119.2		C(01E)	C(01B)	H(01B)	119.8
C(00A)	C(00N)	H(00N)	119.2		C(01D)	C(01C)	C(00Z)	120.17(14)
C(015)	C(00O)	C(00K)	120.98(13)		C(01D)	C(01C)	H(01C)	119.9
C(015)	C(00O)	H(00O)	119.5		C(00Z)	C(01C)	H(01C)	119.9
C(00K)	C(00O)	H(00O)	119.5		C(01C)	C(01D)	C(019)	119.31(13)
C(00W)	C(00P)	C(007)	121.17(11)		C(01C)	C(01D)	H(01D)	120.3
C(00W)	C(00P)	H(00P)	119.4		C(019)	C(01D)	H(01D)	120.3
C(007)	C(00P)	H(00P)	119.4		C(016)	C(01E)	C(01B)	120.68(13)
C(010)	C(00Q)	C(005)	120.28(12)		C(016)	C(01E)	H(01E)	119.7
C(010)	C(00Q)	H(00Q)	119.9		C(01B)	C(01E)	H(01E)	119.7

Table ST3. Bond Lengths for ImPy-3.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
N(001)	C(00G)	1.382(3)		C(00F)	H(00F)	0.9300
N(001)	C(00A)	1.388(3)		C(00G)	C(00J)	1.345(4)
N(001)	C(006)	1.410(3)		C(00G)	H(00G)	0.9300
N(002)	C(00A)	1.319(3)		C(00H)	C(00T)	1.373(4)
N(002)	C(008)	1.385(3)		C(00H)	C(00K)	1.432(4)
C(003)	C(005)	1.397(4)		C(00I)	H(00I)	0.9300
C(003)	C(00D)	1.434(4)		C(00J)	C(00N)	1.420(4)
C(003)	C(009)	1.439(4)		C(00J)	H(00J)	0.9300
C(004)	C(00C)	1.383(4)		C(00K)	H(00K)	0.9300
C(004)	C(00M)	1.432(4)		C(00L)	C(00Q)	1.375(4)
C(004)	C(009)	1.447(4)		C(00L)	H(00L)	0.9300
C(005)	C(00I)	1.371(4)		C(00M)	C(00P)	1.377(5)
C(005)	C(00A)	1.484(4)		C(00M)	H(00M)	0.9300
C(006)	C(008)	1.379(4)		C(00N)	H(00N)	0.9300
C(006)	C(00F)	1.412(4)		C(00O)	C(00S)	1.391(4)
C(007)	C(00O)	1.378(4)		C(00O)	H(00O)	0.9300
C(007)	C(00L)	1.388(4)		C(00P)	H(00P)	0.9300
C(007)	C(008)	1.471(4)		C(00Q)	C(00R)	1.365(5)
C(009)	C(00B)	1.405(4)		C(00Q)	H(00Q)	0.9300
C(00B)	C(00E)	1.416(4)		C(00R)	C(00S)	1.372(5)
C(00B)	C(00H)	1.430(4)		C(00R)	H(00R)	0.9300
C(00C)	C(00I)	1.369(4)		C(00S)	H(00S)	0.9300
C(00C)	H(00C)	0.9300		C(00T)	C(00V)	1.380(5)
C(00D)	C(00K)	1.356(4)		C(00T)	H(00T)	0.9300
C(00D)	H(00D)	0.9300		C(00U)	C(00V)	1.366(5)
C(00E)	C(00U)	1.406(5)		C(00U)	H(00U)	0.9300
C(00E)	C(00P)	1.438(5)		C(00V)	H(00V)	0.9300
C(00F)	C(00N)	1.361(4)				

Table ST4. Bond angles for ImPy-3.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C(008)	N(001)	C(00L)	132.00(10)		C(005)	C(00Q)	H(00Q)	119.9
C(008)	N(001)	C(005)	106.98(10)		C(00X)	C(00R)	C(00K)	120.82(12)
C(00L)	N(001)	C(005)	120.92(10)		C(00X)	C(00R)	H(00R)	119.6
C(00C)	N(002)	C(00U)	132.26(10)		C(00K)	C(00R)	H(00R)	119.6
C(00C)	N(002)	C(009)	107.01(9)		C(012)	C(00S)	C(009)	120.10(12)
C(00U)	N(002)	C(009)	120.64(11)		C(012)	C(00S)	H(00S)	119.9
C(008)	N(003)	C(006)	107.36(10)		C(009)	C(00S)	H(00S)	119.9
C(00C)	N(004)	C(00G)	107.48(10)		C(019)	C(00T)	C(00I)	120.57(13)
C(006)	C(005)	N(001)	105.16(10)		C(019)	C(00T)	H(00T)	119.7
C(006)	C(005)	C(00Q)	136.77(11)		C(00I)	C(00T)	H(00T)	119.7
N(001)	C(005)	C(00Q)	118.00(11)		C(017)	C(00U)	N(002)	119.48(12)
N(003)	C(006)	C(005)	109.95(10)		C(017)	C(00U)	H(00U)	120.3
N(003)	C(006)	C(00I)	122.81(11)		N(002)	C(00U)	H(00U)	120.3
C(005)	C(006)	C(00I)	127.24(10)		C(018)	C(00V)	C(00A)	120.97(13)
C(00H)	C(007)	C(00P)	118.05(11)		C(018)	C(00V)	H(00V)	119.5
C(00H)	C(007)	C(00C)	123.97(12)		C(00A)	C(00V)	H(00V)	119.5
C(00P)	C(007)	C(00C)	117.96(10)		C(00P)	C(00W)	C(00J)	121.61(13)
N(003)	C(008)	N(001)	110.52(10)		C(00P)	C(00W)	H(00W)	119.2
N(003)	C(008)	C(00D)	123.59(11)		C(00J)	C(00W)	H(00W)	119.2
N(001)	C(008)	C(00D)	125.85(11)		C(00R)	C(00X)	C(014)	120.30(13)
C(00G)	C(009)	N(002)	105.23(10)		C(00R)	C(00X)	H(00X)	119.8
C(00G)	C(009)	C(00S)	136.37(12)		C(014)	C(00X)	H(00X)	119.8
N(002)	C(009)	C(00S)	118.37(11)		C(00L)	C(00Y)	C(010)	120.80(13)
C(00N)	C(00A)	C(00V)	122.96(12)		C(00L)	C(00Y)	H(00Y)	119.6
C(00N)	C(00A)	C(00B)	118.13(11)		C(010)	C(00Y)	H(00Y)	119.6
C(00V)	C(00A)	C(00B)	118.91(12)		C(01C)	C(00Z)	C(00I)	121.37(14)
C(00E)-	C(00B)	C(013)	122.26(12)		C(01C)	C(00Z)	H(00Z)	119.3
C(00E)	C(00B)	C(00A)	119.30(11)		C(00I)	C(00Z)	H(00Z)	119.3
C(013)	C(00B)	C(00A)	118.44(11)		C(00Q)	C(010)	C(00Y)	120.17(12)
N(004)	C(00C)	N(002)	110.40(10)		C(00Q)	C(010)	H(010)	119.9
N(004)	C(00C)	C(007)	124.03(12)		C(00Y)	C(010)	H(010)	119.9
N(002)	C(00C)	C(007)	125.56(11)		C(01B)	C(011)	C(00F)	120.95(14)
C(00E)	C(00D)	C(00M)	118.41(11)		C(01B)	C(011)	H(011)	119.5
C(00E)	C(00D)	C(008)	124.16(12)		C(00F)	C(011)	H(011)	119.5
C(00M)	C(00D)	C(008)	117.37(11)		C(00S)	C(012)	C(017)	119.88(13)
C(00D)	C(00E)	C(00B)	121.51(12)		C(00S)	C(012)	H(012)	120.1
C(00D)	C(00E)	H(00E)	119.2		C(017)	C(012)	H(012)	120.1
C(00B)	C(00E)	H(00E)	119.2		C(01A)	C(013)	C(00B)	120.91(13)
C(00H)	C(00F)	C(00J)	119.14(11)		C(01A)	C(013)	H(013)	119.5
C(00H)	C(00F)	C(011)	122.34(12)		C(00B)	C(013)	H(013)	119.5
C(00J)	C(00F)	C(011)	118.51(11)		C(015)	C(014)	C(00X)	119.62(12)
N(004)	C(00G)	C(009)	109.88(10)		C(015)	C(014)	H(014)	120.2
N(004)	C(00G)	C(00K)	121.23(11)		C(00X)	C(014)	H(014)	120.2
C(009)	C(00G)	C(00K)	128.89(11)		C(00O)	C(015)	C(014)	120.30(13)
C(007)	C(00H)	C(00F)	121.90(12)		C(00O)	C(015)	H(015)	119.8

C(007)	C(00H)	H(00H)	119.0		C(014)	C(015)	H(015)	119.8
C(00F)	C(00H)	H(00H)	119.0		C(01E)	C(016)	C(00J)	120.42(15)
C(00T)	C(00I)	C(00Z)	117.72(11)		C(01E)	C(016)	H(016)	119.8
C(00T)	C(00I)	C(006)	121.86(11)		C(00J)	C(016)	H(016)	119.8
C(00Z)	C(00I)	C(006)	120.42(12)		C(00U)	C(017)	C(012)	121.35(13)
C(016)	C(00J)	C(00F)	119.12(12)		C(00U)	C(017)	H(017)	119.3
C(016)	C(00J)	C(00W)	122.83(13)		C(012)	C(017)	H(017)	119.3
C(00F)	C(00J)	C(00W)	118.05(11)		C(00V)	C(018)	C(01A)	120.34(13)
C(00R)	C(00K)	C(00O)	117.96(11)		C(00V)	C(018)	H(018)	119.8
C(00R)	C(00K)	C(00G)	120.37(11)		C(01A)	C(018)	H(018)	119.8
C(00O)	C(00K)	C(00G)	121.62(12)		C(00T)	C(019)	C(01D)	120.82(15)
C(00Y)	C(00L)	N(001)	119.49(12)		C(00T)	C(019)	H(019)	119.6
C(00Y)	C(00L)	H(00L)	120.3		C(01D)	C(019)	H(019)	119.6
N(001)	C(00L)	H(00L)	120.3		C(013)	C(01A)	C(018)	120.41(13)
C(00N)	C(00M)	C(00D)	121.04(12)		C(013)	C(01A)	H(01A)	119.8
C(00N)	C(00M)	H(00M)	119.5		C(018)	C(01A)	H(01A)	119.8
C(00D)	C(00M)	H(00M)	119.5		C(011)	C(01B)	C(01E)	120.30(13)
C(00M)	C(00N)	C(00A)	121.59(12)		C(011)	C(01B)	H(01B)	119.8
C(00M)	C(00N)	H(00N)	119.2		C(01E)	C(01B)	H(01B)	119.8
C(00A)	C(00N)	H(00N)	119.2		C(01D)	C(01C)	C(00Z)	120.17(14)
C(015)	C(00O)	C(00K)	120.98(13)		C(01D)	C(01C)	H(01C)	119.9
C(015)	C(00O)	H(00O)	119.5		C(00Z)	C(01C)	H(01C)	119.9
C(00K)	C(00O)	H(00O)	119.5		C(01C)	C(01D)	C(019)	119.31(13)
C(00W)	C(00P)	C(007)	121.17(11)		C(01C)	C(01D)	H(01D)	120.3
C(00W)	C(00P)	H(00P)	119.4		C(019)	C(01D)	H(01D)	120.3
C(007)	C(00P)	H(00P)	119.4		C(016)	C(01E)	C(01B)	120.68(13)
C(010)	C(00Q)	C(005)	120.28(12)		C(016)	C(01E)	H(01E)	119.7
C(010)	C(00Q)	H(00Q)	119.9		C(01B)	C(01E)	H(01E)	119.7

SI5. Photophysical properties of ImPy derivatives.

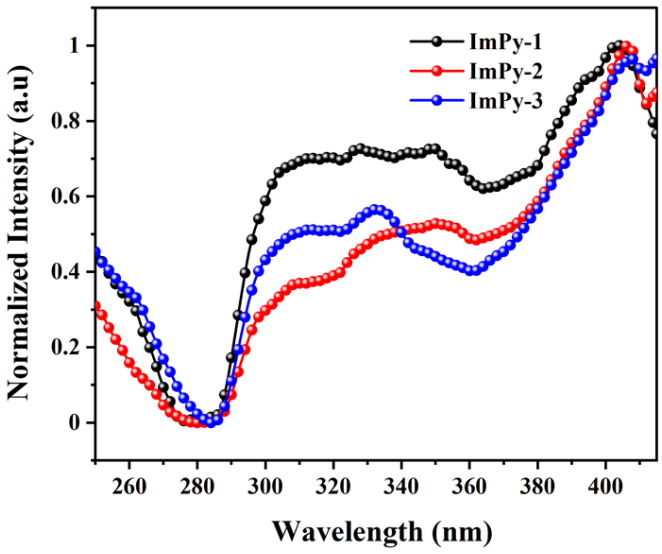


Fig. S10. Normalized PL excitation spectra of the ImPy derivatives in solid states.

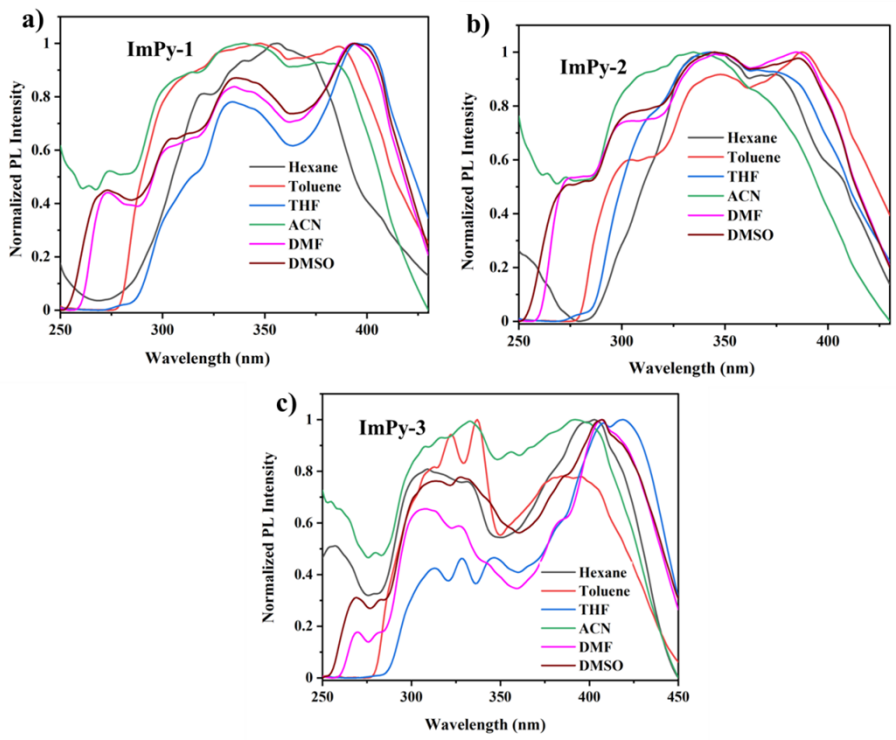


Fig. S11. Normalized PL excitation spectra of the ImPy derivatives in different solvents.

Table ST5. Molar extinction coefficient (ε) data for ImPy-1, ImPy-2 and ImPy-3.

Fluorophores	**λ_{max} (nm)**	**Molar extinction coefficient (ε) cm^{-1}/M**
ImPy-1	234	29656
	291	10705
	360	8734
ImPy-2	293	11501
	313	9602
ImPy-3	255	10687
	297	9928
	356	8354

Table ST6. The CIE color coordinates of ImPy derivatives in solution and solid.

Fluorophores	Solution	Solid
	CIE (x, y)	CIE (x, y)
ImPy-1	(0.20, 0.32)	(0.21, 0.38)

ImPy-2	(0.17, 0.22)	(0.19, 0.37)
ImPy-3	(0.16, 0.22)	(0.25, 0.47)

Table ST7. Fluorescence life time data of ImPy derivatives.

Fluorophore	Excitation wavelength (nm)	Emission wavelength (nm)	Life time (τ) (ns)
ImPy-1	400	489	4.06
ImPy-2	380	462	3.89
ImPy-3	419	477	1.81

SI6. The calculated UV-vis absorption spectra and vertical excitation wavelengths, orbital contribution and oscillator strength (f) of ImPy derivatives.

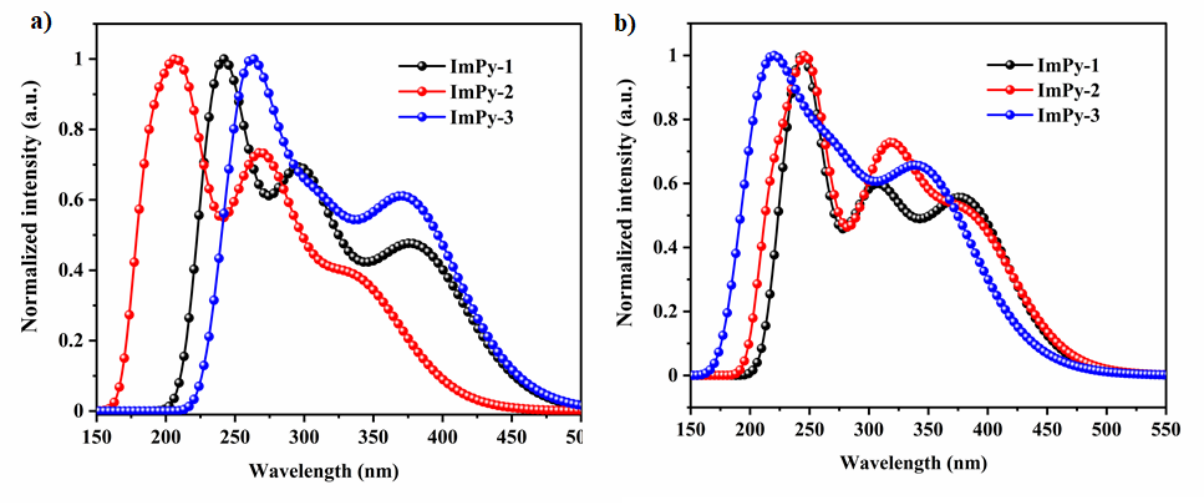


Fig. S12. Simulated UV-vis absorption spectra of the fluorophores Gas and in DCM phase.

Table ST8. The computed vertical transition and their oscillator strengths (*f*) and configuration of the ImPy derivatives

Compound	**State**	**Energy (eV)**	**λ_{max} nm**	***f***	**Configuration**
ImPy-1 Singlet	Gas	3.1636	391.91	0.0582	HOMO → LUMO (52.26%).
		3.2479	381.74	0.2821	HOMO- → LUMO (45.88%). HOMO → LUMO+1 (52.54%).
		3.7940	326.79	0.1617	HOMO → LUMO+1 (66.04%).

		4.1635	297.79	0.3150	HOMO → LUMO+1 (11.19%). HOMO → LUMO+3 (67.56%).
		4.2226	293.62	0.0633	HOMO-1 → LUMO (64.06%). HOMO → LUMO+2 (16.43%).
		4.8793	254.10	0.2248	HOMO-3 → LUMO (27.07%). HOMO-2 → LUMO (16.79%). HOMO → LUMO+5 (54.69%).
	DCM	3.1936	388.23	0.2417	HOMO → LUMO (69.44%).
		3.2624	380.04	0.2840	HOMO- → LUMO+1 (68.64%).
		3.7604	329.71	0.2023	HOMO → LUMO+2 (67.13%).
		4.0640	305.08	0.3608	HOMO → LUMO+3 (68.26%).
		4.2228	293.61	0.0916	HOMO-1 → LUMO (64.21%). HOMO → LUMO+2 (16.54%).
		4.3115	287.57	0.0365	HOMO → LUMO+4 (67.59%).
		4.9111	252.46	0.4987	HOMO-1 → LUMO (64.21%). HOMO → LUMO+2 (16.54%).
		5.1100	242.63	0.2420	HOMO-5 → LUMO (13.68%). HOMO-4 → LUMO (26.12%). HOMO-1 → LUMO+2 (26.55%). HOMO-1 → LUMO+3 (15.89%). HOMO → LUMO+4 (23.52%). HOMO → LUMO+5 (31.70%).
Triplet	GAS	2.2394	553.65	0	HOMO → LUMO+1 (50.99%).
	DCM	2.3041	538.10	0	HOMO → LUMO (57.37%).
ImPy-2 Singlet	Gas	3.1045	399.36	0.0464	HOMO → LUMO (51.98%).
		3.2005	387.39	0.2704	HOMO → LUMO (45.87%). HOMO → LUMO+1 (52.36%).
		3.7897	327.16	0.3072	HOMO → LUMO+2 (66.19%).
		4.0919	303.00	0.3696	HOMO → LUMO+2 (11.71%). HOMO → LUMO+3 (63.67%).
		4.7285	262.21	0.1265	HOMO-2 → LUMO+1 (56.76%).
		4.8172	257.38	0.1744	HOMO-2→ LUMO (15.18%). HOMO-2 → LUMO+1 (14.98%). HOMO-1 → LUMO+2 (29.75%).

					HOMO → LUMO+5 (57.26%).
		4.9511	250.42	0.2161	HOMO-3 → LUMO (16.90%). HOMO-3 → LUMO+1 (32.65%). HOMO → LUMO+5 (20.07%).
		5.4500	227.49	0.1730	HOMO-2 → LUMO+2 (49.42%). HOMO-1 → LUMO+3 (12.82%).
	DCM	3.1536	393.15	0.1573	HOMO → LUMO (66.66%).
		3.2067	386.64	0.3373	HOMO → LUMO (21.04%). HOMO → LUMO+1 (66.07%).
		3.7433	331.22	0.3921	HOMO → LUMO+2 (67.35%).
		3.9901	310.73	0.2941	HOMO → LUMO+3 (47.43%).
		4.7988	258.36	0.4124	HOMO-2 → LUMO+1 (43.47%).
		4.9565	250.14	0.1066	HOMO-2→ LUMO (17.54%). HOMO-1 → LUMO+2 (14.40%). HOMO-1 → LUMO+3 (54.28%).
		5.0620	244.93	0.3585	HOMO-4→ LUMO (14.13%). HOMO-3 → LUMO (34.87%). HOMO-1 → LUMO+3 (26.63%). HOMO → LUMO+5 (19.69%). HOMO → LUMO+6 (24.61%).
Triplet	Gas	2.2075	561.66	0	HOMO-1 → LUMO+1 (16.34%). HOMO → LUMO (47.58%).
	DCM	2.2721	545.69	0	HOMO-1 → LUMO+1 (53.11%).
ImPy-3 Singlet	Gas	2.8094	441.32	0.3120	HOMO → LUMO (69.29%).
		3.4551	358.84	0.1168	HOMO-2 → LUMO (23.50%). HOMO → LUMO+2 (56.20%).
		3.6144	343.03	0.1775	HOMO-2 → LUMO (18.09%). HOMO-1→ LUMO (58.02%). HOMO → LUMO+2 (27.80%).
		4.0571	305.60	0.0993	HOMO→ LUMO+3 (56.40%). HOMO→ LUMO+4 (33.90%).
		4.1097	301.69	0.1421	HOMO-1 → LUMO+4 (11.35%). HOMO → LUMO+4 (57.42%).
		4.4451	278.92	0.1718	HOMO-1→ LUMO+2 (15.48%).

					HOMO → LUMO+5 (25.06%). HOMO → LUMO+6 (54.51%).
		4.4868	276.33	0.0879	HOMO-4 → LUMO (11.56%). HOMO-3 → LUMO (45.71%). HOMO-2 → LUMO (29.17%).
		4.7533	260.84	0.0876	HOMO-1 → LUMO+4 (51.59%). HOMO-1 → LUMO+5 (12.31%).
	DCM	2.7506	450.76	0.4291	HOMO → LUMO (69.85%).
		3.1998	387.48	0.1310	HOMO → LUMO+1 (69.06%).
		3.4390	360.53	0.1577	HOMO-2 → LUMO (20.94%). HOMO → LUMO+2 (54.88%).
		3.5930	345.07	0.2296	HOMO-2 → LUMO (17.22%). HOMO-1 → LUMO (57.08%). HOMO → LUMO+2 (32.55%).
		4.0076	309.38	0.2295	HOMO → LUMO+3 (48.51%). HOMO → LUMO+4 (13.54%).
		4.0491	306.20	0.1167	HOMO-1→ LUMO+4 (11.64%). HOMO → LUMO+4 (64.82%).
		4.3810	283.00	0.2366	HOMO-5 → LUMO (22.61%). HOMO-4 → LUMO (21.49%). HOMO-1 → LUMO+2 (37.93%). HOMO → LUMO+6 (35.19%).
		4.4927	275.97	0.1154	HOMO-5 → LUMO (30.85%). HOMO-4 → LUMO (36.80%). HOMO → LUMO+6 (19.33%).
Triplet	Gas	1.9708	629.12	0	HOMO-1 → LUMO (40.22%). HOMO → LUMO (55.16%).
	DCM	1.9783	626.72	0	HOMO-1 → LUMO (40.85%). HOMO → LUMO (55.12%).

SI7. Atoms coordinates of ImPy-1, ImPy-2 and ImPy-3.

ImPy-1

6 1.9030290 1.3192920 0.0378780

6	2.6430130	2.5226130	-0.0472520
6	2.0065750	3.7294340	0.0439190
6	0.5943490	3.7731090	0.2462730
6	-0.1345700	2.6281650	0.2850830
6	0.0112960	0.1106910	0.1288250
6	2.1831520	-0.0532280	0.0167750
1	3.7129160	2.4651080	-0.1926880
1	2.5675670	4.6526560	-0.0272300
1	0.0851210	4.7197280	0.3714070
1	-1.1999870	2.6020060	0.4497420
7	1.0162020	-0.7501700	0.0687630
7	0.4959890	1.4070260	0.1311320
6	3.4752870	-0.7423090	-0.0842300
6	4.6690530	-0.1774690	0.3909760
6	3.5274320	-2.0248250	-0.6540240
6	5.8767710	-0.8601290	0.2744070
1	4.6517370	0.7837500	0.8900080
6	4.7336360	-2.7057150	-0.7639020
1	2.6061230	-2.4719570	-1.0053680
6	5.9167130	-2.1251090	-0.3069990
1	6.7865540	-0.4071810	0.6530890
1	4.7521980	-3.6937700	-1.2107840
1	6.8574130	-2.6567650	-0.3952380
6	-1.3959020	-0.2897770	0.1981170
6	-2.4297510	0.4314290	-0.3726220
6	-1.6963600	-1.5259810	0.8432980
6	-3.7732720	-0.0157830	-0.3013770
1	-2.2297300	1.3377610	-0.9320310
6	-2.9839660	-1.9816590	0.9251590
1	-0.8757520	-2.0942720	1.2613740
6	-4.8427780	0.7139770	-0.8842130
6	-4.0635110	-1.2457300	0.3670420
1	-3.1952490	-2.9214600	1.4247300
6	-6.1353650	0.2558000	-0.8011400
1	-4.6233170	1.6436550	-1.3993330
6	-5.4076350	-1.6890860	0.4376790
6	-6.4218910	-0.9564080	-0.1317890
1	-6.9426530	0.8233680	-1.2501820
1	-5.6239860	-2.6217150	0.9483090
1	-7.4461160	-1.3067120	-0.0723700

ImPy-2

6	2.6886610	1.2879040	-0.0911460
6	3.4884230	2.4516650	-0.1848730

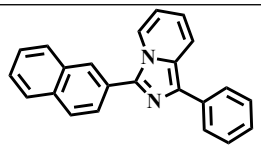
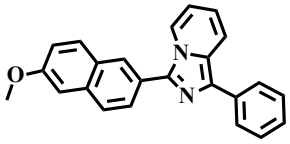
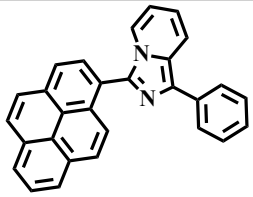
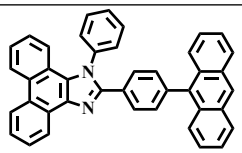
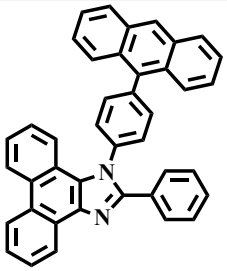
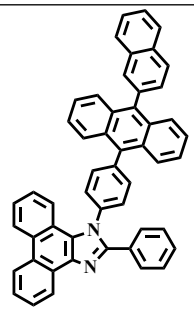
6	2.9072360	3.6733990	-0.3830760
6	1.4900880	3.7715170	-0.5202770
6	0.7092530	2.6633340	-0.4435320
6	0.7489330	0.1545750	-0.1622110
6	2.9080430	-0.0908670	0.0232850
1	4.5629440	2.3496500	-0.1236660
1	3.5169710	4.5646790	-0.4605810
1	1.0203520	4.7280260	-0.7087760
1	-0.3595230	2.6738880	-0.5859870
7	1.7155320	-0.7433500	-0.0461660
7	1.2873560	1.4292690	-0.2091540
6	4.1699760	-0.8245750	0.1753250
6	5.3012850	-0.2577050	0.7828960
6	4.2554740	-2.1508110	-0.2786350
6	6.4842400	-0.9813270	0.9044120
1	5.2485320	0.7407080	1.1995780
6	5.4360630	-2.8722120	-0.1514770
1	3.3794770	-2.6010020	-0.7280650
6	6.5603230	-2.2899750	0.4338810
1	7.3443620	-0.5248490	1.3820720
1	5.4808220	-3.8940320	-0.5124090
1	7.4814670	-2.8534390	0.5306140
6	-0.6748860	-0.1827030	-0.2253060
6	-1.6750110	0.6006530	0.3201590
6	-1.0357920	-1.4216180	-0.8368620
6	-3.0379520	0.2155750	0.2531220
1	-1.4345110	1.5118090	0.8557470
6	-2.3414980	-1.8190480	-0.9149750
1	-0.2431400	-2.0420490	-1.2344870
6	-4.0752810	1.0032280	0.8064100
6	-3.3905250	-1.0167450	-0.3831200
1	-2.5942760	-2.7617510	-1.3886150
6	-5.3927850	0.6131160	0.7335140
1	-3.8213350	1.9361180	1.2992230
6	-4.7452910	-1.3986330	-0.4515820
6	-5.7358780	-0.6039300	0.0936200
1	-6.1585470	1.2414000	1.1679070
1	-5.0295660	-2.3279880	-0.9311990
8	-7.0147260	-1.0636390	-0.0247500
6	-8.0756690	-0.3024530	0.5349920
1	-8.1500580	0.6889760	0.0743870
1	-8.9844360	-0.8631430	0.3224600
1	-7.9665270	-0.1935120	1.6197810

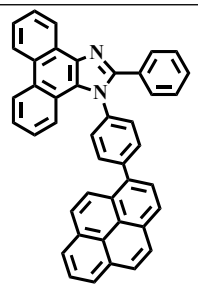
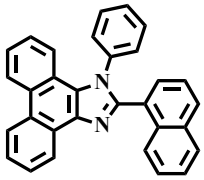
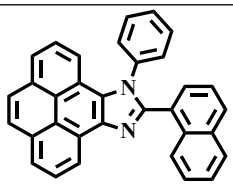
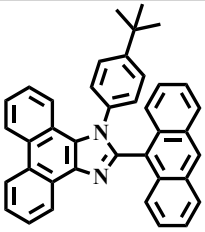
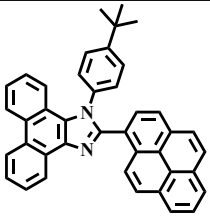
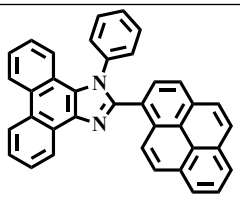
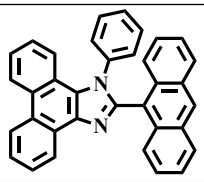
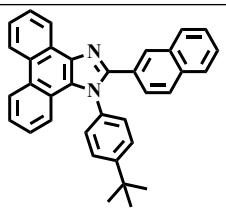
ImPy-3

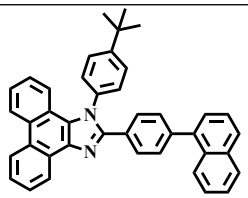
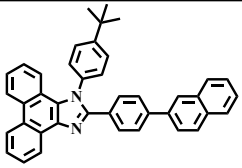
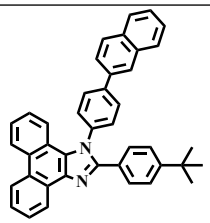
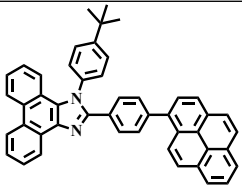
6	-5.2538660	-2.9241600	-1.3170070
6	-3.8909270	-2.7977180	-1.5751160
6	-3.1536070	-1.7305710	-1.0362250
6	-3.8158060	-0.7700700	-0.2145180
6	-5.2148810	-0.9081730	0.0436250
6	-5.9107700	-1.9909820	-0.5172560
6	-1.7506150	-1.5633740	-1.2826820
6	-3.0842110	0.3236970	0.3434000
6	-1.6828300	0.4606960	0.0824890
6	-1.0488020	-0.5235400	-0.7534130
6	-0.9838230	1.5667030	0.6394240
6	-1.6819740	2.4815300	1.4470900
6	-3.0395880	2.3473620	1.7007570
6	-3.7675980	1.2785220	1.1578340
6	-5.1727370	1.1138660	1.4020420
6	-5.8649660	0.0696540	0.8707470
1	-6.9284290	-0.0421060	1.0646170
1	-5.6752720	1.8477410	2.0264500
1	-1.2467390	-2.2940790	-1.9098740
1	-5.8086350	-3.7554170	-1.7421170
1	-3.3830690	-3.5277520	-2.1995170
1	-6.9743700	-2.0940790	-0.3198180
1	0.0143050	-0.4346250	-0.9357150
1	-1.1369240	3.2968320	1.9128500
1	-3.5455230	3.0665270	2.3390190
6	2.4168820	2.8008300	0.0220130
7	1.4064960	0.8466680	0.5326200
7	1.0198160	2.9921720	0.0937030
6	2.6124080	1.4377240	0.2888600
6	3.8612020	0.6685570	0.3573390
6	3.9123520	-0.4944250	1.1473040
6	5.0135140	1.0394170	-0.3578410
6	5.0813810	-1.2447430	1.2342500
1	3.0204780	-0.7930500	1.6873940
6	6.1849530	0.2893220	-0.2626880
1	4.9851380	1.8955640	-1.0237800
6	6.2270630	-0.8536150	0.5364860
1	5.1006170	-2.1374570	1.8531960
1	7.0625410	0.5921330	-0.8270470
1	7.1394420	-1.4383050	0.6085130
6	2.6587010	5.1512640	-0.4858950
1	3.2785920	6.0197120	-0.6799390
6	1.2350710	5.2798910	-0.4960230
1	0.7681310	6.2294800	-0.7310620

6	3.2315710	3.9317810	-0.2374190
1	4.3077140	3.8104130	-0.2248190
6	0.4571490	1.7670390	0.4194880
6	0.4423360	4.2119950	-0.2084570
1	-0.6382090	4.2431010	-0.2012800

Table ST 9. Summary of performance of reported purely organic small molecules unipolar blue OLEDs so far voltage (OV), power efficiency (PE), current efficiency (CE), external quantum efficiency (EQE), and CIE coordinates of the devices.

Emitters	**Voltage [V]**	**PE_{max} lm W^{-1}**	**CE_{max} cd A^{-1}**	**EQE_{max} (%)**	**CIE (x, y)**	**Ref.**
	7.5	0.8	2.5	1.2	(0.19, 0.24)	This work
	6.2	1.9	3.7	1.6	(0.21, 0.32)	This work
	**5.6**	**4.7**	**8.4**	**4.3**	**(0.19, 0.36)**	**This work**
	2.76	3.03	4.36	3.52	0.156, 0.155	[2]
	3.74	1.01	2.41	1.56	0.166, 0.213	[3]
	3.32	1.51	3.24	2.71	0.154, 0.147	

	3.59	1.76	3.64	2.82	0.153, 0.163	
	3.8	-	0.513	2.43	0.160, 0.034	[4]
	2.9	-	2.62	3.68	0.157, 0.084	
	2.6	0.71	1.15	0.83	0.16, 0.17	[5]
	2.5	0.49	0.90	0.85	0.15, 0.12	
	3.2	-	5.88	5.11	0.15, 0.14	[6]
	3.5	-	3.43	2.29	0.16, 0.18	
	2.8	0.78	0.89	0.95	0.15, 0.11	[7]

	3.2	0.55	0.53	0.60	0.14, 0.10	
	3.0	1.44	1.37	1.61	0.14, 0.11	
	3.4	1.07	1.2	1.47	0.15, 0.11	
	2.5	3.17	3.27	2.07	0.15, 0.18	

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