Supporting Informaiton

A Novel Design Strategy of Tetradentate Pt(II) Complexes through Conformation Manager for High Efficiency and Narrow Emission in Blue Organic Light-Emitting Diodes

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1. General information

All chemical compounds were commercially available. Reaction reagents were purchased from Sigma Aldrich Co., Alfa aesar Co., and TCI Co. Paldium catalysts were puchased from P&H Tech Co. Solvents were purchased from Samchun Pure Chemical CO., Ltd., Duksan Sci. Co., and Daejung Chemical & Metal Co. ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were measured on Unity Inova 500 MHz spectrometer. Chloroform-d_3 ($CDCl_3$) and methylene chloride-d_2 (CD_2Cl_2) were used for NMR analysis. UV-vis spectrophometer (JASCO, V-730) and fluorescence spectopheometer (PerkinElmer, LS-55) were used for UV-vis spectra and PL spectra, respectrively. The HOMO levels were estimated using a cyclic voltammetry (CV) (Ivium Tech., Iviumstat). CV measurement was carried out in dichloromethane solution with scan rate at 100 mV/s. The platinum wires were used as working and counter and Ag/AgCl was used as reference electrode respectively. Internal standard was ferrocenium/ferrocene couple and supporting electrolyte was 0.1 M tetrabutylammonium perchlorate ($TBAClO_4$). The mass spectra were measured using a JMS-700 (JEOL) with high resolution fast atom bombardment (FAB) mode and Advion Expression-L CMS spectrometer in APCI mode. PL quantum yield and transient PL decay data were obtained using Quantaurus QY Absolute system (Hamamatsu, C11347-11) and Hamamatsu Quantaurus-Tau system (Hamamatsu, C11367-31). The thermal stability was measured using Seiko Exstar 6000 (TG/DTA6100) for thermogravimetric analyzer (TGA) and Nexta DSC 600 for differential Scanning Calorimetry analysis (DSC). The sample was heated at a rate of 10 °C/min to 600 °C under an N_2 atmosphere in the TGA measurement. The sample was heated at a rate of 10 °C/min from 0 °C to 350 °C in the DSC measurement.

2. Computational details

Density functional theory (DFT) calculations and time-dependent DFT (TD-DFT) were performed using the Gaussian 16 program package. The ground state geometries were optimized using B3LYP functional and LANL2DL basis set for Pt and B3LYP/6-31g(d,p) for light elements (C, H, N and O). The computations of the singlet and triplet transition energies were carried out using TD-DFT by same method based on the optimized ground state geometry.[1]

3. Experimental Procedures

1-(3-bromophenyl)-4-methyl-1*H*-benzo[*d*]imidazole (Me-L2)

4-Methyl-1*H*-benzo[*d*]imidazole (1.32 g, 10 mmol), 1-bromo-3-fluorobenzene (1.7 mL, 15 mmol) and potassium phosphate tribasic (K_3PO_4) (10 g, 50 mmol) were added into a two-neck flask. *N,N*-dimethylformamide (20 mL) was added into the flask. The flask was stirred at 160 °C for 12 h. After completion of the reaction, the reaction mixture was slowly cooled to room temperature. The product was extracted using methylene chloride (MC) and water. A white solid was obtained after further purification by column chromatography using ethyl acetate (EA):hexane (1:4) eluent (1.8 g, yield 62%). ^{1}H NMR (500 MHz, CD_3Cl): δ 8.20 (s, 1H), 7.69 (td, J = 1.9, 0.5 Hz, 1H), 7.61 (dt, J = 7.2, 1.8 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.37 (ddd, J = 8.2, 1.1, 0.6 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.21 – 7.17 (m, 1H), 2.74 (s, 3H). MS (APCI) m/z 287.0 [$(M+H)^+$].

9-(4-(tert-butyl)pyridin-2-yl)-2-(3-(4-methyl-1*H*-benzo[*d*]imidazol-1-yl)phenoxy)-9*H*-carbazole (Me-L1)

Me-L2 (1.7 g, 6.0 mmol), 9-(4-(*tert*-butyl)pyridin-2-yl)-9*H*-carbazol-2-ol[2] (2.1 g, 6.6 mmol), copper iodide (I) (0.3 g, 1.8 mmol), picolinic acid (1.2 g, 9.6 mmol), and K_3PO_4 (5.1 g, 24 mmol) were added and dissolved in dimethyl sulfoxide (DMSO) (12 mL) into a two-neck flask. After that, the flask was stirred at 100 °C for 12 h. When the reaction finished, the residue was filtered using EA at short silica column. The filtrate was extracted using EA and washed by brine. A brown powder was obtained after further purification by column chromatography using an EA:hexane (1:4) eluent (2.3 g, yield 73%). ^{1}H NMR (500 MHz, CD_3Cl): δ 8.57 (dd, J = 5.3, 0.6 Hz, 1H), 8.17 (s, 1H), 8.11 – 8.08 (m, 1H), 8.08 – 8.06 (m, 1H), 7.72 (dt, J = 8.3, 0.8 Hz, 1H), 7.60 – 7.59 (m, 1H), 7.57 (dd, J = 1.7, 0.7 Hz, 1H), 7.50 – 7.46 (m, 1H), 7.42 (ddd, J = 8.4, 7.2, 1.2 Hz, 1H), 7.40 – 7.36 (m, 1H), 7.34 – 7.30 (m, 1H), 7.27 (dd, J = 5.4, 1.7 Hz, 1H), 7.23 – 7.18 (m, 3H), 7.15 – 7.12 (m, 1H), 7.11 (ddd, J = 8.3, 2.3, 0.9 Hz, 1H), 7.08 (dd, J = 8.4, 2.2 Hz, 1H), 2.71 (s, 3H), 1.35 (s, 9H). MS (APCI) m/z 523.2 [$(M+H)^+$].

9-(4-(*tert*-butyl)pyridin-2-yl)-2-(3-(3-(3,5-di-*tert*-butylphenyl)-4-methyl-1*H*-3λ^4-benzo[*d*]imidazol-1-yl)phenoxy)-9*H*-carbazole trifluoromethanesulfonate (Me-L)

Me-L1 (3.4 g, 5.7 mmol), (3,5-di-*tert*-butylphenyl)(mesityl)iodonium trifluoromethane sulfonate[3] (2.0 g, 3.8 mmol) and copper acetate (41.8 mg, 0.2 mmol) were added into a two-neck flask and dissolved in dimethylformamide (19 mL). The flask was stirred at 130 °C at 12 h. After that, filtered roughly through a short pad of silica and washed with EA:MC (1/9) eluent.

Brown powder was obtained without further purification and used it next metalation (3.1 g, yield 94%).

Platinum(II) 1-(3-((9-(4-(*tert*-butyl)pyridin-2-yl-*κ*N)-9*H*-carbazol-2-yl-*κ*C^1)oxy)phenyl-*κ*C^1)-3-(3,5-di-*tert*-butylphenyl)-4-methyl-1*H*-benzo[*d*]imidazol-2-ylidene-*κ*C^2 (Pt-Me-bzim)

Me-L (2.0 g, 2.3 mmol), dichloro(1,5-cyclooctadiene)platinum(II) (Pt(cod)Cl$_2$) (0.9 g, 2.3 mmol), and sodium acetate (NaOAc) (0.6 g, 7.0 mmol) were added it into a two-neck flask and dissolved in DMF (40 mL). The flask was stirred at 160 °C for 12 h. After that, the reaction was extracted using MC and water. A yellow powder was obtained after further purification by column chromatography using an MC:hexane (1:1) eluent (850 mg, yield 41%). ^{1}H NMR (500 MHz, CD$_2$Cl$_2$): δ 8.61 (d, J = 6.3 Hz, 1H), 8.07 (s, J = 8.3 Hz, 1H), 8.04 – 8.00 (m, 1H), 7.79 (d, J = 1.9 Hz, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.61 – 7.57 (m, 1H), 7.50 (d, J = 1.5 Hz, 2H), 7.40 – 7.35 (m, 2H), 7.35 – 7.31 (m, 2H), 7.30 (d, J = 8.2 Hz, 1H), 7.26 (t, J = 7.9 Hz, 1H), 7.07 (d, J = 5.0 Hz, 1H), 7.06 – 7.04 (m, 1H), 6.11 (dd, J = 6.3, 2.0 Hz, 1H), 1.85 (s, 3H), 1.46 (s, 9H), 1.13 (s, 18H). ^{13}C NMR (125MHz, CD$_2$Cl$_2$) δ 190.2, 162.1, 155.0, 154.2, 152.6, 150.4, 148.4, 144.2, 138.9, 137.8, 134.9, 132.5, 128.9, 126.7, 124.5, 124.4, 123.9, 123.0, 122.3, 119.9, 116.1, 115.4, 114.2, 113.6, 112.3, 112.2, 109.7, 108.1, 35.2, 31.2, 29.8, 19.0. HRMS (FAB+) m/z 904.3565 [(M+H)$^+$]. Calculated for $C_{49}H_{48}N_4OPt$: 903.3476.

4-bromo-1-(3-iodophenyl)-1*H*-benzo[*d*]imidazole (Ph-L3)

Ph-L3 was synthesized by using the same method for synthesis of **Me-L2**. 4-Bromo-1H-benzo[*d*]imidazole (7.4 g, 37.3 mmol) was used and a product was obtained after further purification by column chromatography using an EA/hexane (1:4) eluent (7.1 g, yield 48%). ^{1}H NMR (500 MHz, CD_3Cl): δ 8.14 (s, 1H), 7.87 (t, J = 1.8 Hz, 1H), 7.84 (dd, J = 7.9, 0.9 Hz, 1H), 7.55 (d, J = 7.7 Hz, 1H), 7.49 (ddd, J = 8.0, 2.0, 0.8 Hz, 1H), 7.46 (d, J = 8.2 Hz, 1H), 7.32 (t, J = 8.0 Hz, 1H), 7.22 (t, J = 8.0 Hz, 1H). MS (APCI) m/z 398.9 [$(M+H)^+$].

2-(3-(4-bromo-1*H*-benzo[*d*]imidazol-1-yl)phenoxy)-9-(4-(*tert*-butyl)pyridin-2-yl)-9*H*-carbazole (Ph-L2)

Ph-L2 was synthesized by using the same method for synthesis of **Me-L1**. **Ph-L3** (7.0 g, 17.5 mmol) was used and a product was obtained after further purification by column chromatography using an EA/hexane (1:4) eluent (6.3 g, yield 61%). ^{1}H NMR (500 MHz, CD_3Cl): δ 8.58 (d, J = 5.3 Hz, 1H), 8.16 (s, 1H), 8.10 (t, J = 8.1 Hz, 2H), 7.73 (d, J = 8.3 Hz, 1H), 7.61 (d, J = 2.1 Hz, 1H), 7.58 (d, J = 1.5, 1H), 7.52 – 7.47 (m, 3H), 7.46 – 7.41 (m, 1H), 7.33 (t, J = 7.4 Hz, 1H), 7.29 (d, J = 5.3, 1.7 Hz, 1H), 7.21 (t, J = 2.1 Hz, 1H), 7.17 (dd, J = 16.1, 8.0 Hz, 2H), 7.13 (dd, J = 8.4, 2.3 Hz, 1H), 7.08 (dd, J = 8.4, 2.1 Hz, 1H), 1.36 (s, 9H). MS (APCI) m/z 587.1 [$(M+H)^+$].

9-(4-(tert-butyl)pyridin-2-yl)-2-(3-(4-phenyl-1H-benzo[d]imidazol-1-yl)phenoxy)-9H-carbazole (Ph-L1)

Ph-L2 (2.0 g, 3.4 mmol), phenylboronic acid (0.5 g, 4.0 mmol), tris(dibenzylideneacetone)dipalladium ($Pd_2(dba)_3$) (0.3 g, 0.3 mmol), XPhos (0.5 g, 1.0 mmol) and K_3PO_4 (2.2 g, 10.2 mmol) were added and dissolved in toluene (7 mL)/1,4-dioxane/water (2:1:1) into a two-neck flask. The flask was stirred at 100 °C for 12 h. After that, the product was extracted using MC and water. A pale yellow powder was obtained after further purification by column chromatography using a EA:hexane (1:4) eluent (2.0 g, yield 98%). ^{1}H NMR (500 MHz, CD_3Cl): δ 8.59 (dd, J = 5.3, 0.6 Hz, 1H), 8.26 (s, 1H), 8.13 – 8.10 (m, 1H), 8.09 (ddd, J = 7.8, 1.2, 0.7 Hz, 1H), 7.95 (dd, J = 8.2 Hz, 2H), 7.73 (dd, J = 4.8, 4.1 Hz, 1H), 7.62 (d, J = 2.1 Hz, 1H), 7.59 (dd, J = 1.7, 0.6 Hz, 1H), 7.54 (dt, J = 2.4, 1.3 Hz, 2H), 7.51 (dt, J = 3.8, 1.7 Hz, 2H), 7.48 (dd, J = 7.5, 1.0 Hz, 1H), 7.44 (ddd, J = 8.4, 7.2, 1.3 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.37 – 7.31 (m, 1H), 7.29 (dd, J = 5.4, 1.7 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.24 (ddd, J = 7.8, 2.0, 0.9 Hz, 1H), 7.14 (ddd, J = 8.4, 2.4, 0.8 Hz, 1H), 7.11 (dd, J = 8.4, 2.2 Hz, 1H), 1.37 (s, 9H). MS (APCI) m/z 585.3 $[(M+H)^+]$.

9-(4-(*tert*-butyl)pyridin-2-yl)-2-(3-(3-(3,5-di-*tert*-butylphenyl)-4-phenyl-1*H*-3λ^4-benzo[*d*]imidazol-1-yl)phenoxy)-9*H*-carbazole trifluoromethanesulfonate (Ph-L)

Ph-L was synthesized by using the same method for synthesis of **Me-L**. **Ph-L1** (0.2 g, 0.3 mmol) was used and a product was filtered roughly through a short pad of silica and washed with EA:MC (1:9) eluent. Brown powder was obtained without further purification and used it next metalation (0.25 g, yield 82%).

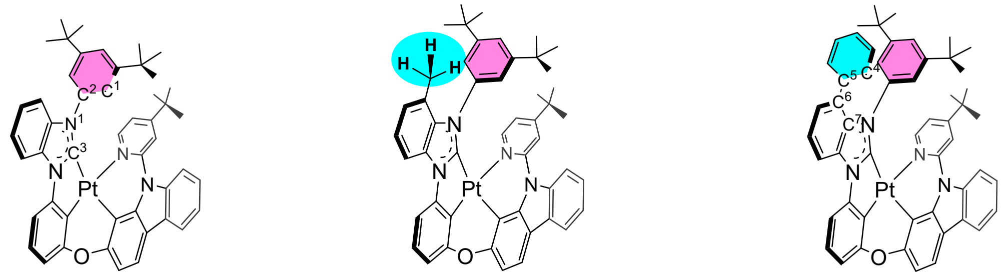
Platinum(II) 1-(3-((9-(4-(*tert*-butyl)pyridin-2-yl-*κ*N)-9*H*-carbazol-2-yl-*κ*C^1)oxy)phenyl-*κ*C^1)-3-(3,5-di-*tert*-butylphenyl)-4-phenyl-1*H*-benzo[*d*]imidazol-2-ylidene-*κ*C^2 (Pt-Ph-bzim)

Pt-Ph-bzim was synthesized by using the same method for synthesis of **Pt-Me-bzim**. **Me-L** (600 mg, 0.65 mmol) was used and a product was obtained after further purification by column chromatography using an MC:hexane (1:1) eluent (440 mg, yield 35%).

^{1}H NMR (500 MHz, CD_2Cl_2): δ 8.37 (d, J = 6.3 Hz, 1H), 8.27 (dd, J = 8.4, 0.9 Hz, 1H), 8.06 – 8.01 (m, 1H), 7.79 (d, J = 8.2 Hz, 1H), 7.73 (d, J = 1.8 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.70 (dd, J = 7.7, 0.9 Hz, 1H), 7.59 (s, 1H), 7.52 (dd, J = 8.3, 7.6 Hz, 2H), 7.41 – 7.36 (m, 1H), 7.36 – 7.26 (m, 5H), 7.22 (dd, J = 7.5, 0.9 Hz, 1H), 7.07 (dd, J = 8.1, 0.9 Hz, 1H), 7.01 (t, J = 1.7 Hz, 1H), 7.00 – 6.97 (m, 1H), 6.79 (s, 1H), 6.47 (d, J = 84.3 Hz, 1H), 5.95 (dd, J = 6.3, 2.0 Hz, 1H), 1.10 (s, 18H), 1.04 (s, 9H). ^{13}C NMR (125MHz, CD_2Cl_2) δ 191.3, 162.0, 154.8, 154.0, 152.3, 150.5, 148.5, 144.3, 138.9, 137.6, 137.2, 133.2, 133.1, 126.7, 124.41, 124.38, 123.8, 123.2, 122.3, 122.0, 119.9, 116.2, 115.64, 115.55, 115.5, 114.1, 113.7, 112.4, 112.2, 110.7, 108.0, 35.1, 34.6, 31.3, 29.7. HRMS (FAB+) m/z 966.3708 $[(M+H)^+]$. Calculated for $C_{54}H_{50}N_4OPt$: 965.3633.

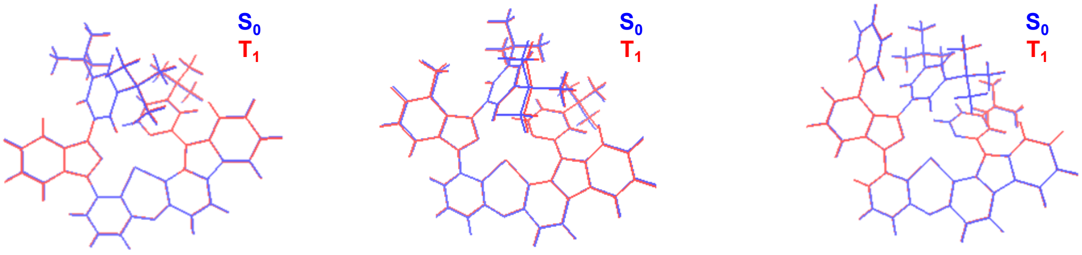
4. Supplementary Figures

(a)



	BD-02	**Pt-Me-bzim**	**Pt-Ph-bzim**	
	∠C^1-C^2-N^1-C^3 (°)	∠C^1-C^2-N^1-C^3 (°)	∠C^1-C^2-N^1-C^3 (°)	∠C^4-C^5-C^6-C^7 (°)
S_0	54.856	68.470	64.697	58.187
T_1	51.689	67.758	64.188	54.794
S_0-T_1	3.167	0.712	0.509	3.393

(b)



0.119 Å **0.179 Å** **0.116 Å**

Figure S1. (a) The details of calculated geometries. (b) Root mean square displacement (RMSD) of **BD-02**, **Pt-Me-bzim** and **Pt-Ph-bzim**.

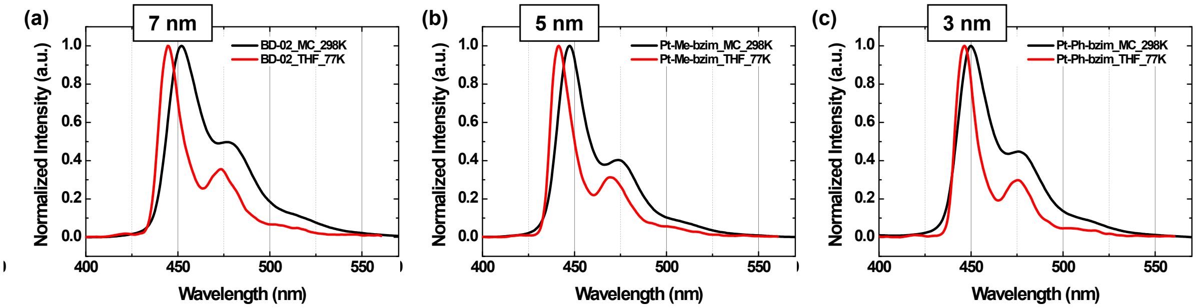


Figure S2. PL spectra of (a) **BD-02**, (b) **Pt-Me-bzim**, and (c) **Pt-Ph-bzim** at 298 and 77 K.

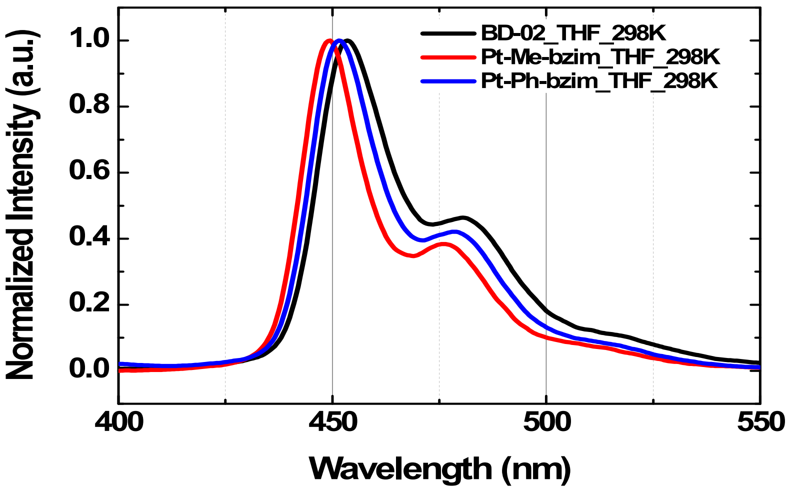


Figure S3. PL spectra of BD-02, Pt-ME-bzim, and Pt-Ph-bzim on THF solution (1.0 × 10^{-5} M) at 298K

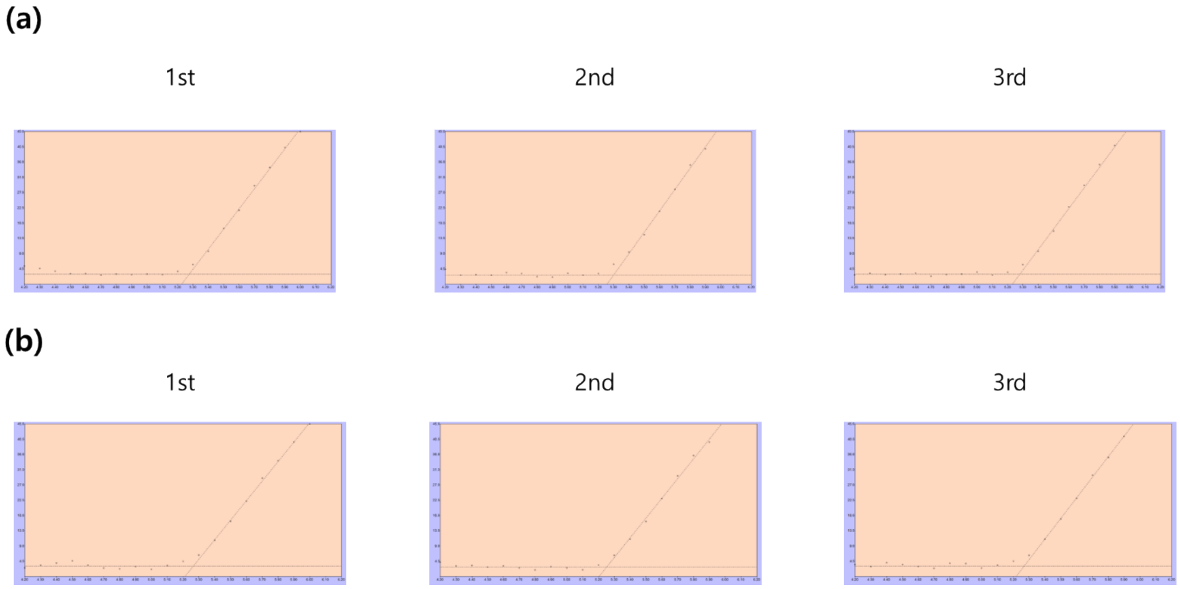


Figure S4. Photoemission yield spectroscopy in air measurement of (a) Pt-ME-bzim and (b) Pt-Ph-bzim in air measurements

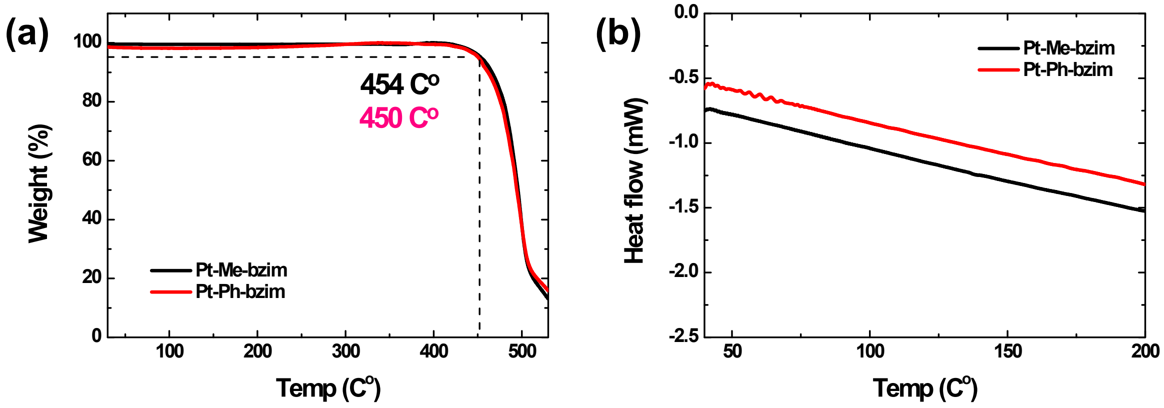


Figure S5. (a) TGA and (b) DSC measurements for **Pt-Me-bzim** and **Pt-Ph-bzim** (DSC measurements: 2nd scan after N_2 treatment, 10 °C min^{-1}, under N_2).

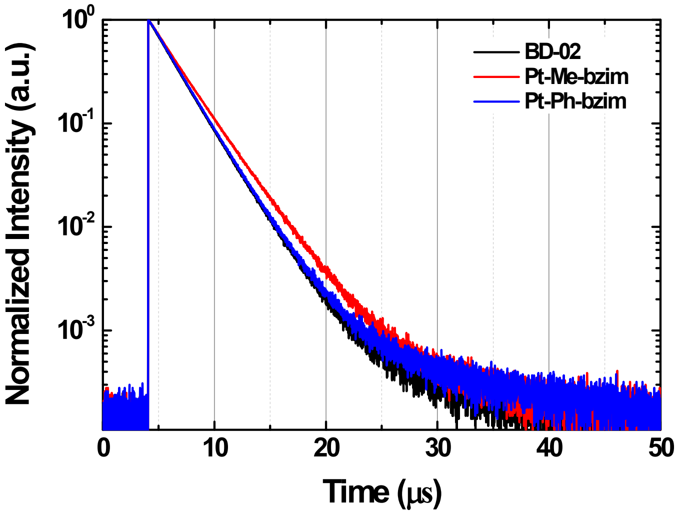


Figure S6. TRPL curves of (a) **BD-02**, (b) **Pt-Me-bzim**, and (c) **Pt-Ph-bzim**.

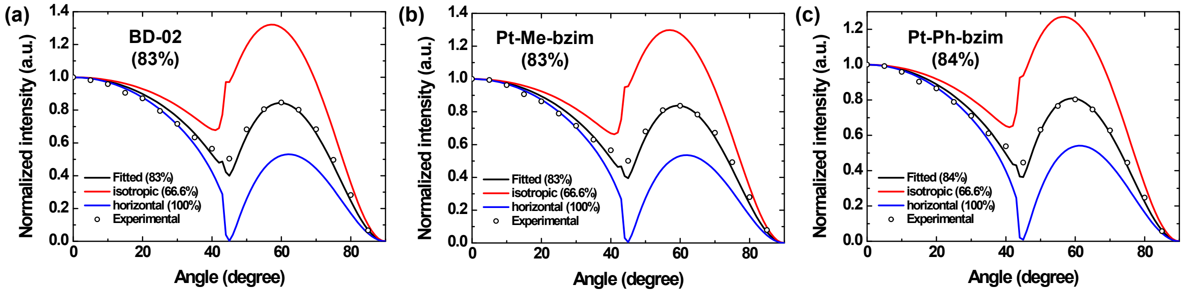


Figure S7. ADPL curves of (a) **BD-02**, (b) **Pt-Me-bzim**, and (c) **Pt-Ph-bzim**.

Figure S8. (a) Energy diagram of PhOLEDs with **BD-02**, **Pt-Me-bzim**, and **Pt-Ph-bzim**. (b) The molecular structure of materials used for fabricating PhOLEDs.

Figure S9. (a) EL spectra, (b) *J-V-L* curves, and (c) luminance-EQE curves of PhOLEDs based on **BD-02**, **Pt-Me-bzim**, and **Pt-Ph-bzim** at 15 and 20 wt% doping concentration.

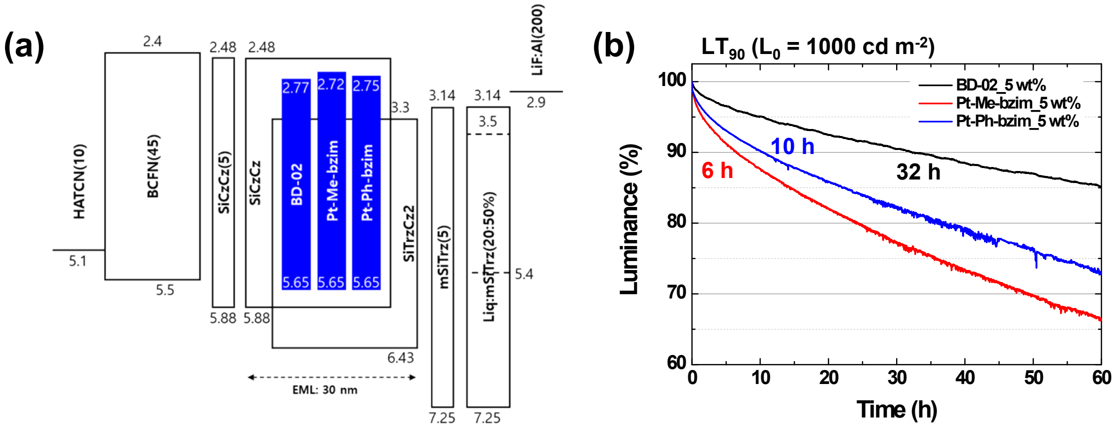


Figure S10. (a) Energy diagram of PhOLEDs with **BD-02**, **Pt-Me-bzim**, and **Pt-Ph-bzim**. (b) operational lifetime curves of PhOLEDs.

5. Supplementary Tables

Table S1. HOMO levels measured from phtoemission yield spectroscopy in air(PYSA) measurments

Sample	HOMO [eV]		
	1st	2nd	3rd
Pt-Me-bzim	-5.28	-5.30	-5.28
Pt-Ph-bzim	-5.26	-5.25	-5.27

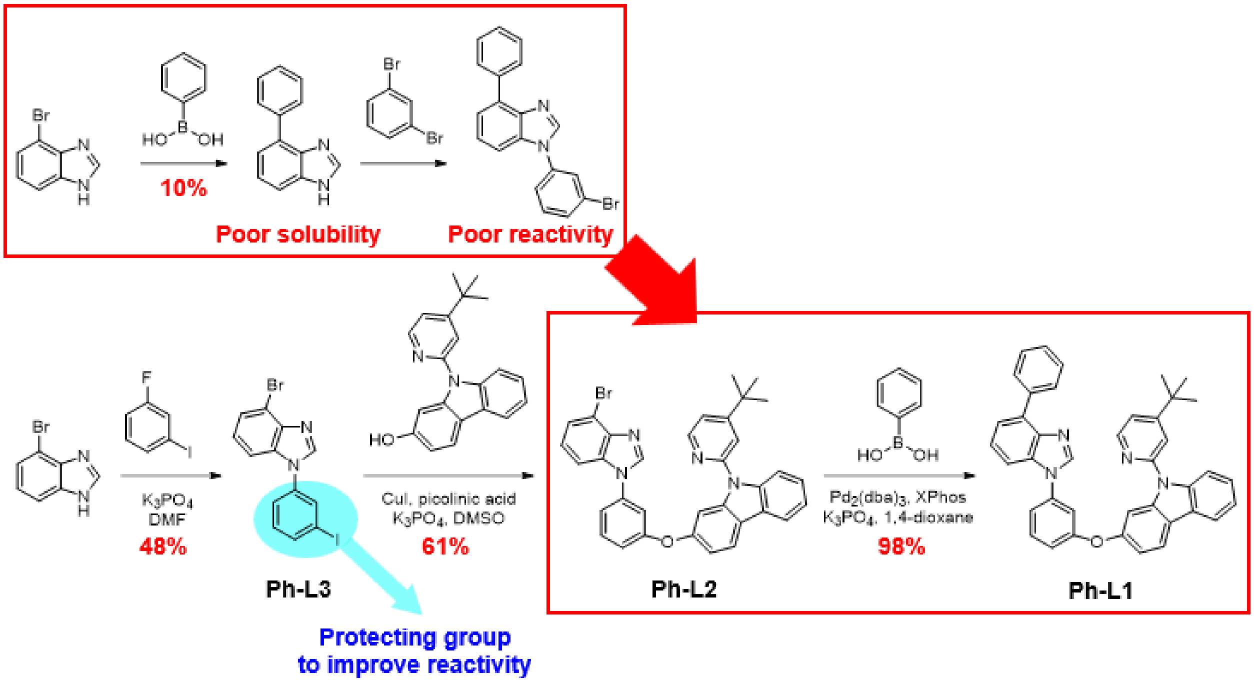
Table S2. Summarized EQE, CIE_y, and FWHM of tetradentate Pt(II) complexes

Pt dopant	EQE_{max} (%)	CIE_y	FWHM (nm)	ref
Pt-Me-bzim	**27.1**	**0.084**	**18**	**This work**
Pt-Ph-bzim	**27.5**	**0.100**	**20**	**This work**
BD-02 (PtON-TBBI)	25.2	0.115	21	This work
PtON1	23.3	0.13	-	4
PtON7	20.4	0.14	-	4
PtON7-dtb	24.8	0.079	29	5
PtON1-tBu	5.3	0.098	24	5
PtON6-tBu	10.9	0.093	30	5
Pt7O7	26.3	0.24	-	6
6	15.4	0.17	-	7
10	17.6	0.29	-	8
11	15.6	0.28	-	8
PtSN1	14.4	0.48	-	9
PtSN2	36.2	0.47	-	9
Pt-Ada	20.6	0.11	-	10

Pt-R	21.4	0.12	-	10
Pt-AdaPh	21.2	0.12	-	10
Pt-AdaTol	22.6	0.122	-	10
PtON7-TMS	21.4	0.097	30	11
t-Pt-Ad	20.3	0.092	-	12
Pt-NPT	19.8	0.118	-	12
Pt-adNPT	15.7	0.090	-	12
Pt-tmCyCz	21.5	0.13	22	13
Pt-tBuCz	23.7	0.172	25	2
Pt-dipCz	25.0	0.157	22	2
Pt-biPh	19.0	0.15	21	14
Pt-biPh5tBu	18.1	0.168	22	14
Pt-biPh4tBu	21.8	0.149	21	14
PtON-tb-DTB	20.9	0.22	-	15
PtON-tb-TTB	26.7	0.22	-	15
Pt3	20.2	0.181	-	16
Pt4	21.0	0.175	-	16
PtON5N-dtb	20.4	0.17	30	17

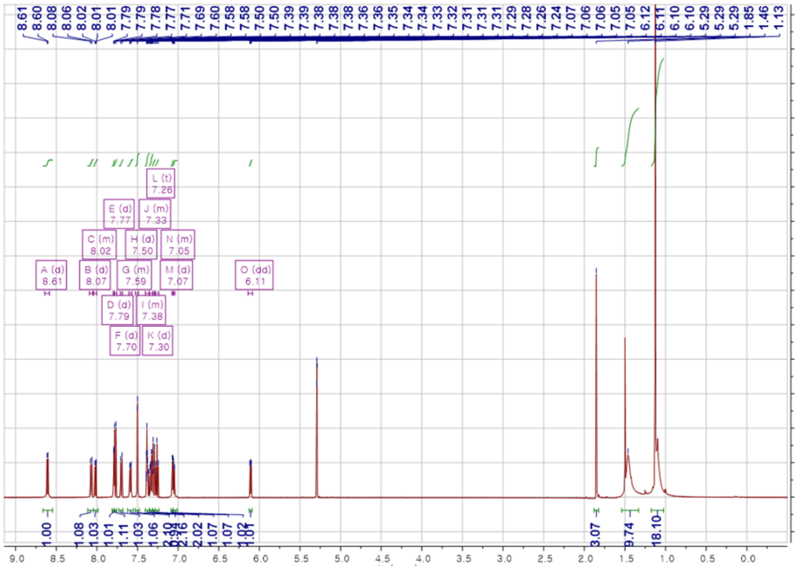
Pt-SPCz	25.1	0.131	22	18
Pt(t-BuBnOCzPy)	19.0	0.17	26	19
Pt(BnOCz4t-BuPy)	18.6	0.17	26	19
PtON7-dtb	27.6	0.088	28	20
BD-02 (PtON-TBBI)	28.0	0.104	21	20

6. Supplementary Scheme

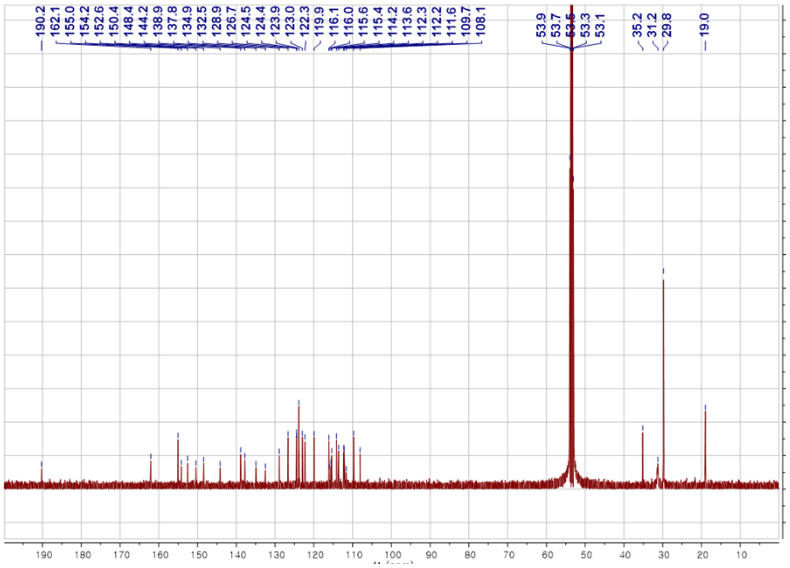


Scheme S1. Improved synthetic scheme of **Pt-Ph-bzim**.

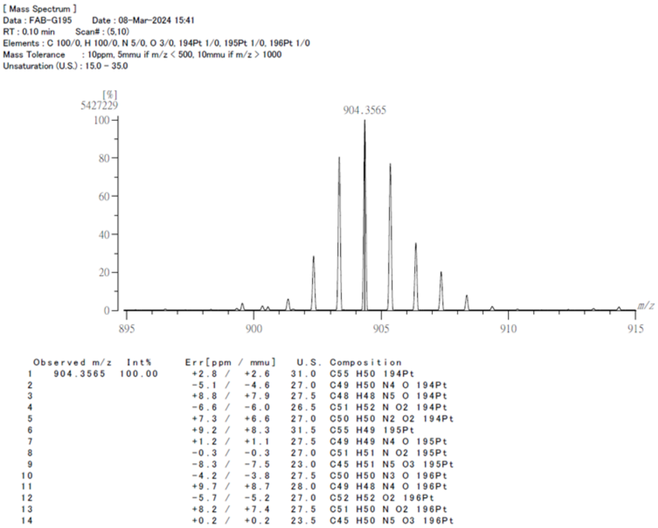
7. ^{1}H, ^{13}C NMR and HRMS



^{1}H NMR data of **Pt-Me-bzim**.



^{13}C NMR data of **Pt-Me-bzim**.



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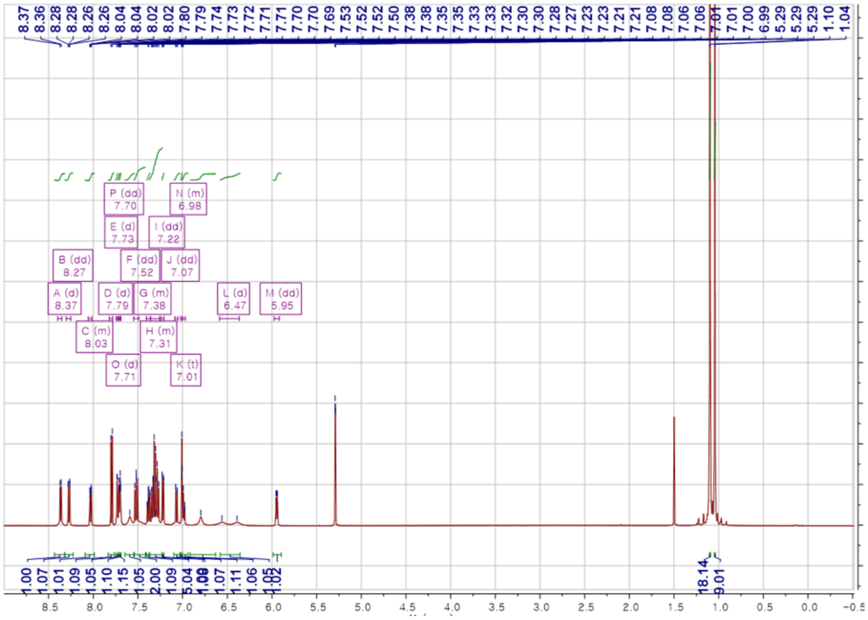
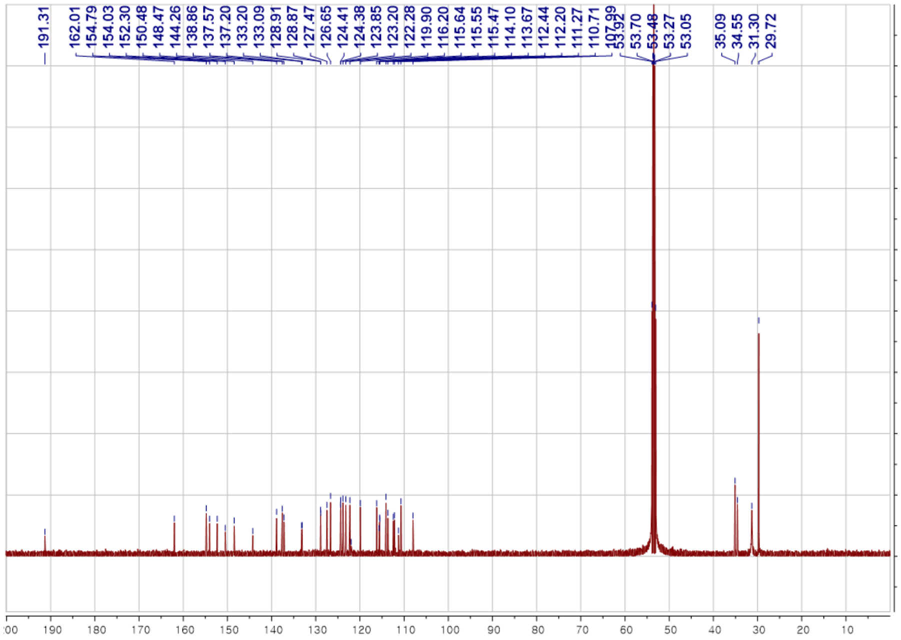
[ Mass Spectrum ]
Data : FAB-G195      Date : 08-Mar-2024 15:41
RT : 0.10 min      Scan# : (5,10)
Elements : C 100/0, H 100/0, N 5/0, O 3/0, 194Pt 1/0, 195Pt 1/0, 196Pt 1/0
Mass Tolerance     : 10ppm, 5mmu if m/z < 500, 10mmu if m/z > 1000
Unsaturation (U.S.) : 15.0 - 35.0
```

```
 Observed m/z  Int%      Err[ppm / mmu]   U.S.  Composition
 1   904.3565  100.00      +2.8 /  +2.6   31.0  C55 H50 194Pt
 2                         -5.1 /  -4.6   27.0  C49 H50 N4 O 194Pt
 3                         +8.8 /  +7.9   27.5  C48 H48 N5 O 194Pt
 4                         -6.6 /  -6.0   26.5  C51 H52 N O2 194Pt
 5                         +7.3 /  +6.6   27.0  C50 H50 N2 O2 194Pt
 6                         +9.2 /  +8.3   31.5  C55 H49 195Pt
 7                         +1.2 /  +1.1   27.5  C49 H49 N4 O 195Pt
 8                         -0.3 /  -0.3   27.0  C51 H51 N O2 195Pt
 9                         -8.3 /  -7.5   23.0  C45 H51 N5 O3 195Pt
10                         -4.2 /  -3.8   27.5  C50 H50 N3 O 196Pt
11                         +9.7 /  +8.7   28.0  C49 H48 N4 O 196Pt
12                         -5.7 /  -5.2   27.0  C52 H52 O2 196Pt
13                         +8.2 /  +7.4   27.5  C51 H50 N O2 196Pt
14                         +0.2 /  +0.2   23.5  C45 H50 N5 O3 196Pt
```

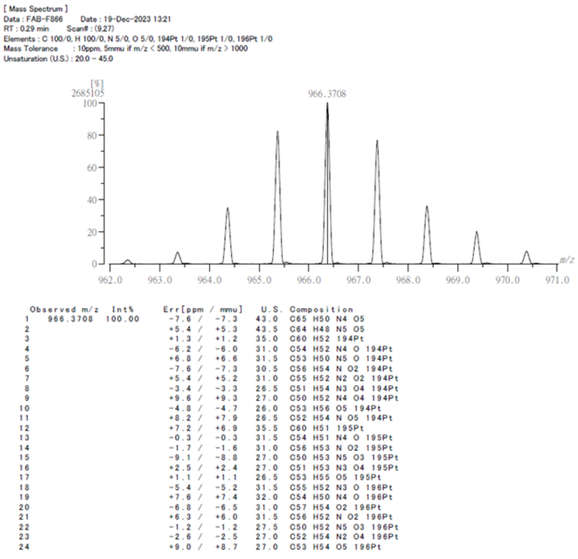
HRMS data of **Pt-Me-bzim**.



^{1}H NMR data of **Pt-Ph-bzim**.



^{13}C NMR data of **Pt-Me-bzim**.



```
[ Mass Spectrum ]
Data : FAB-F866       Date : 19-Dec-2023 13:21
RT : 0.29 min       Scan# : (9,27)
Elements : C 100/0, H 100/0, N 5/0, O 5/0, 194Pt 1/0, 195Pt 1/0, 196Pt 1/0
Mass Tolerance       : 10ppm, 5mmu if m/z < 500, 10mmu if m/z > 1000
Unsaturation (U.S.) : 20.0 - 45.0
```

```
  Observed m/z  Int%      Err[ppm / mmu]   U.S.  Composition
 1   966.3708  100.00      -7.6 /  -7.3   43.0  C65 H50 N4 O5
 2                         +5.4 /  +5.3   43.5  C64 H48 N5 O5
 3                         +1.3 /  +1.2   35.0  C60 H52 194Pt
 4                         -6.2 /  -6.0   31.0  C54 H52 N4 O 194Pt
 5                         +6.8 /  +6.6   31.5  C53 H50 N5 O 194Pt
 6                         -7.6 /  -7.3   30.5  C56 H54 N O2 194Pt
 7                         +5.4 /  +5.2   31.0  C55 H52 N2 O2 194Pt
 8                         -3.4 /  -3.3   26.5  C51 H54 N3 O4 194Pt
 9                         +9.6 /  +9.3   27.0  C50 H52 N4 O4 194Pt
10                         -4.8 /  -4.7   26.0  C53 H56 O5 194Pt
11                         +8.2 /  +7.9   26.5  C52 H54 N O5 194Pt
12                         +7.2 /  +6.9   35.5  C60 H51 195Pt
13                         -0.3 /  -0.3   31.5  C54 H51 N4 O 195Pt
14                         -1.7 /  -1.6   31.0  C56 H53 N O2 195Pt
15                         -9.1 /  -8.8   27.0  C50 H53 N5 O3 195Pt
16                         +2.5 /  +2.4   27.0  C51 H53 N3 O4 195Pt
17                         +1.1 /  +1.1   26.5  C53 H55 O5 195Pt
18                         -5.4 /  -5.2   31.5  C55 H52 N3 O 196Pt
19                         +7.6 /  +7.4   32.0  C54 H50 N4 O 196Pt
20                         -6.8 /  -6.5   31.0  C57 H54 O2 196Pt
21                         +6.3 /  +6.0   31.5  C56 H52 N O2 196Pt
22                         -1.2 /  -1.2   27.5  C50 H52 N5 O3 196Pt
23                         -2.6 /  -2.5   27.0  C52 H54 N2 O4 196Pt
24                         +9.0 /  +8.7   27.0  C53 H54 O5 196Pt
```

HRMS data of **Pt-Me-bzim**.

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