Supporting Information

Rhodium-Catalyzed Annulation between 2-Arylimidazo[1, 2-a]pyridines and Alkynes Leading to Pyrido[1,2-a]benzi-midazole Derivatives

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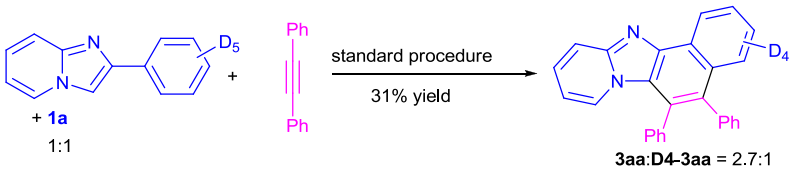
1 General experimental details

Chemicals were used as received without special purification unless stated otherwise. ^{1}H and ^{13}C NMR spectra were recorded at ambient temperature on a 300 or 400 MHz NMR spectrometer (75 or 100 MHz for ^{13}C NMR). NMR results were reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (δ 7.26 or 77.0 ppm) as the internal standard. The coupling constants *J* are given in Hz. Melting points were taken on an electrothermal melting point apparatus and without correction. IR spectra were recorded on a spectrometer using KBr discs. $[Cp^*Rh(MeCN)_3](SbF_6)_2$ was prepared according to literature procedure,[1] stored in a dessicator and weighed out to air. D_5-acetophenone was prepared through literature method.[2]

2. Mechanistic Experiments

2.1 The KIE studies on 2-phenylimidazo[1,2-a]pyridine

In a sealed tube, the mixture of **1a**/ **D_5-1a** (1: 1, 0.2 mmol), **2a** (0.24 mmol) was treated under standard conditions for 2 h. After that, the mixture was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with dichloromethane-ethyl acetate as eluent to give product **3aa** and **D_4-3aa**. The mixture was analyzed using ^{1}H NMR spectrometer. As shown in Figure S1, the ratio of **3aa** and **D_{11}-3aa** is nearly 2.7.



Scheme S1 KIE experiment of **1a** and **D_4-1a.**

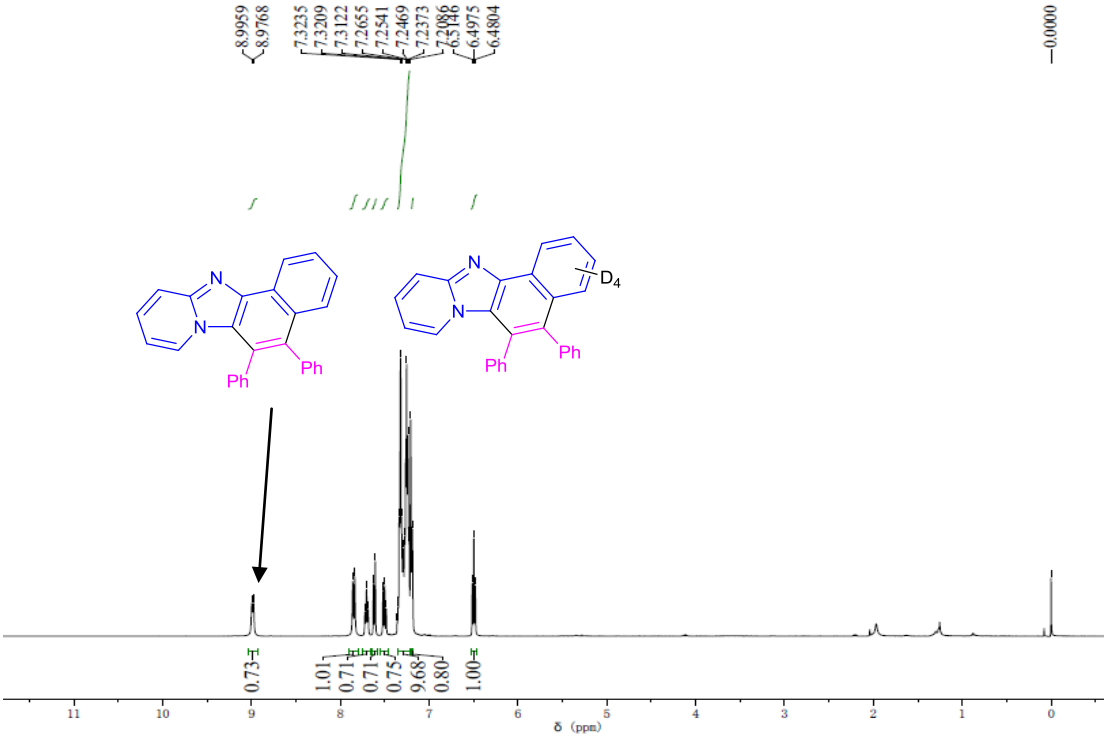


Figure S1 The ^{1}H NMR spectrum of the KIE results.

2.2 Deuterium kinetic isotope effect (DKIE) measurements.

Under air, a sealed reaction tube was charged with **1a** (0.2 mmol), D_2O (25.0 equiv), [Cp*Rh(MeCN)$_3$](SbF$_6$)$_2$ (2.5 mol %), $Cu(OAc)_2$ (1.2 equiv) and 1.5 mL of toluene. The reaction mixture was stirred at 110 ^{o}C for 12 h. After the completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on a silica gel to give the product. The mixture was analyzed using ^{1}H NMR spectrometer. The results are shown in Figure S2.

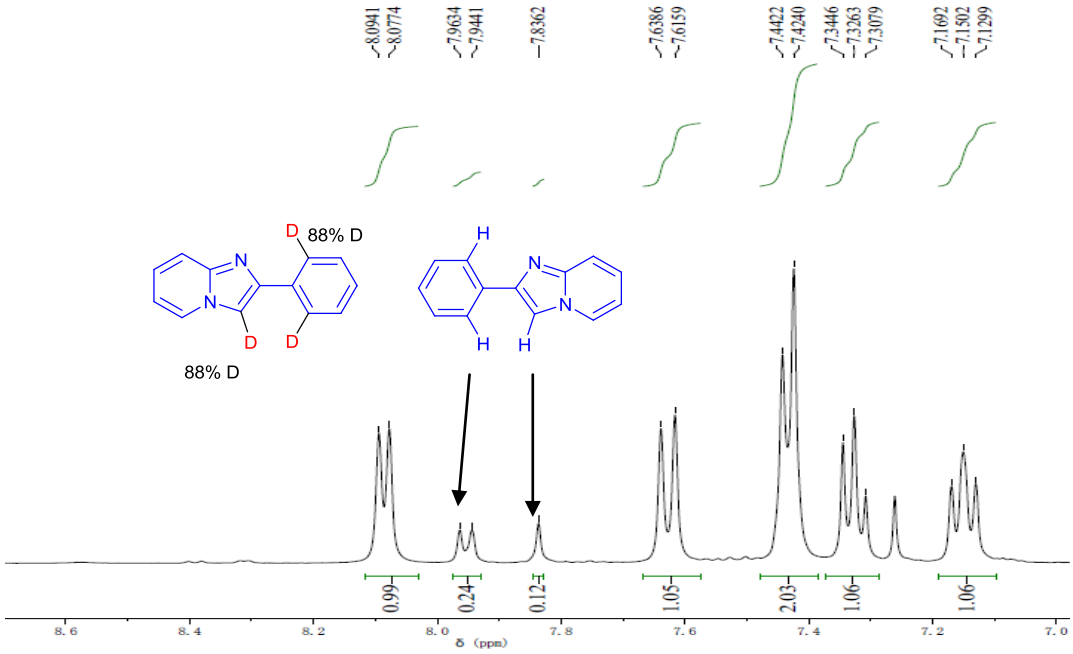
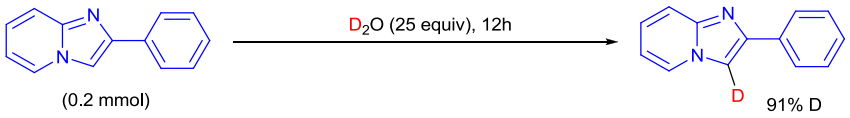


Figure S2



Under air, a sealed reaction tube was charged with **1a** (0.2 mmol), D_2O (25.0 equiv) and 1.5 mL of toluene. The reaction mixture was stirred at 110 ^{o}C for 12 h. After the completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on a silica gel to give the product. The mixture was analyzed using ^{1}H NMR spectrometer. The results are shown in Figure S3.

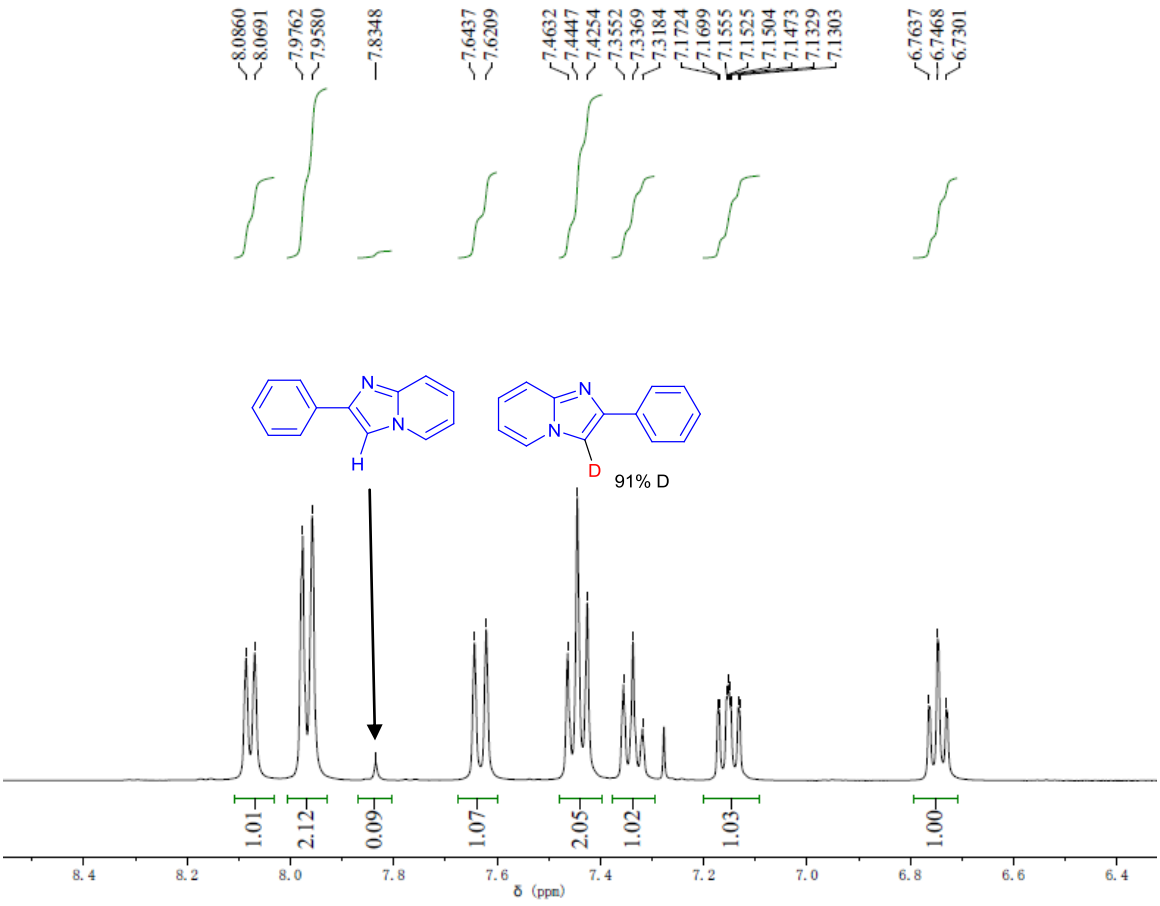
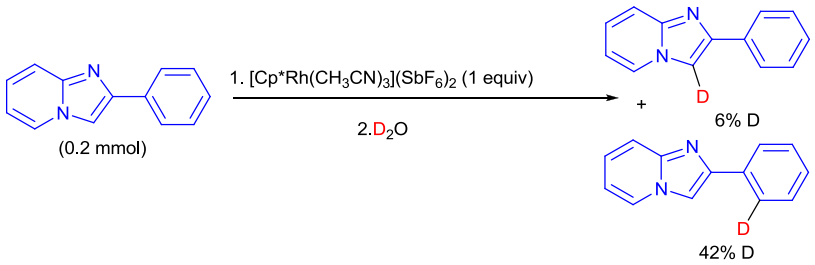


Figure S3



Under air, a sealed reaction tube was charged with **1a** (0.2 mmol), [Cp*Rh(MeCN)3](SbF6)2 (1equiv) and 1.5 mL of toluene. The reaction mixture was stirred at 110 °C for 12 h then quenched by D_2O (25.0 equiv). After the completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on a silica gel to give the product. The mixture was analyzed using ^1H NMR spectrometer. As shown in Figure S4.

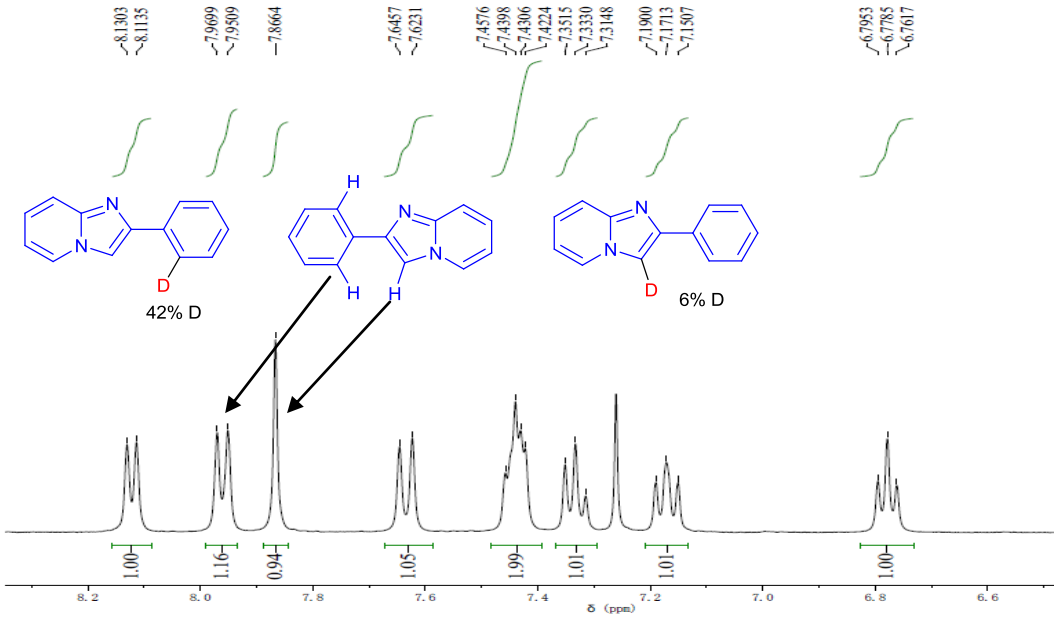


Figure S4

3 UV-Vis Absorption and Fluorescence

3.1 UV-Vis Absorption Spectra of 3aa and 3ga.

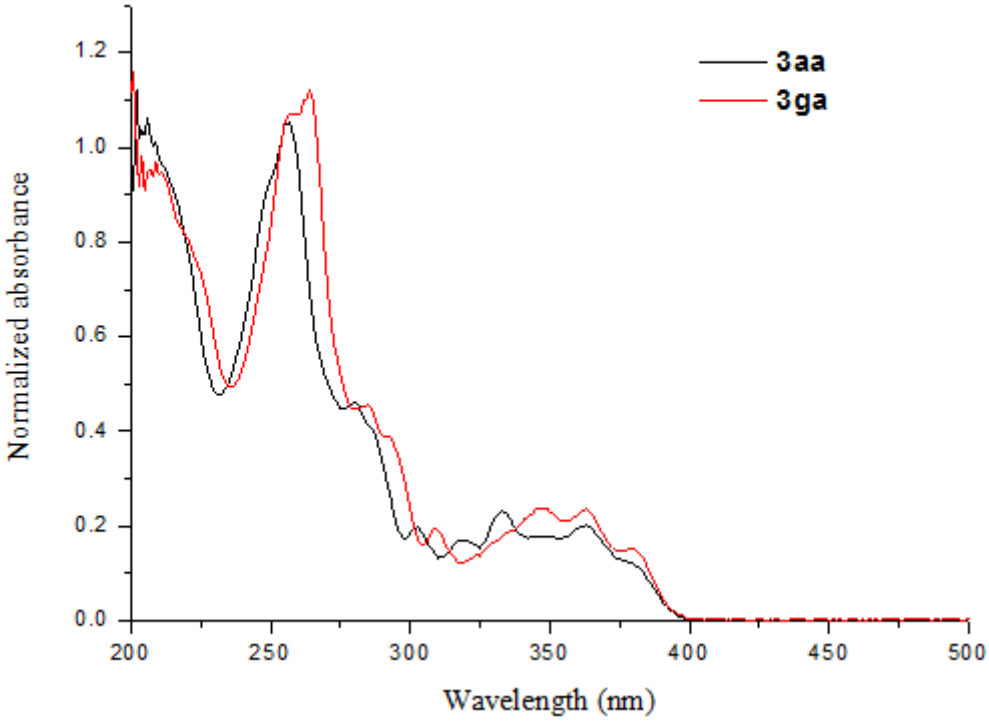


Figure S5 UV-vis absorption spectra of **3aa** and **3ga** in CH_3OH.

3.2 Fluorescence Spectra of 3aa and 3ga.

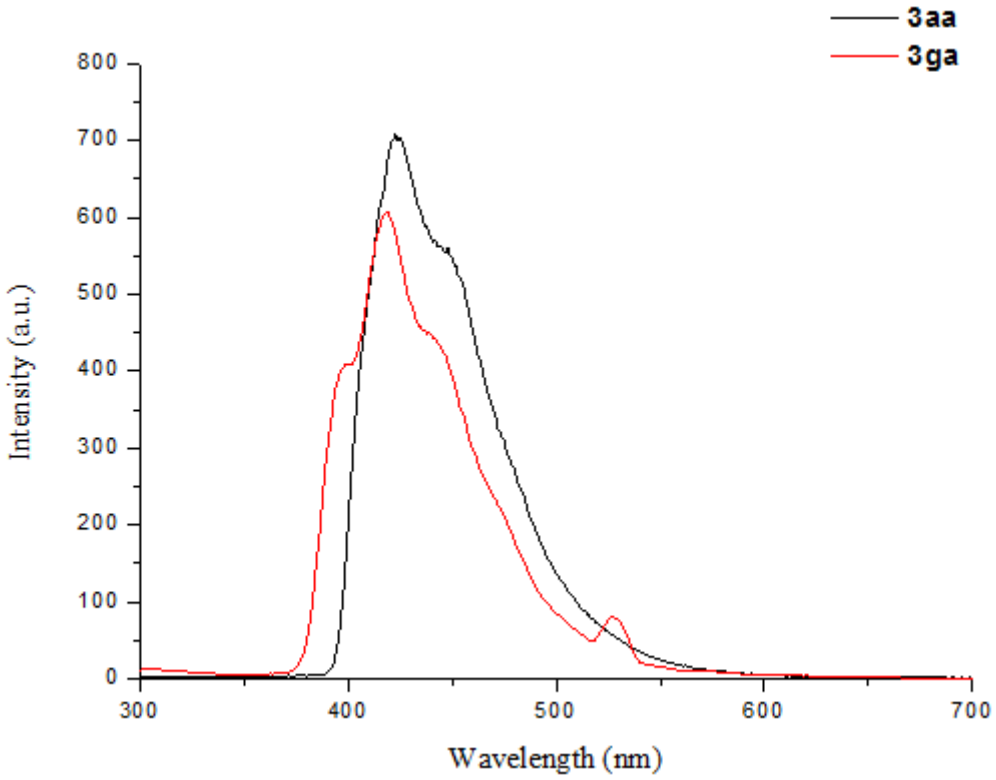


Figure S6 Fluorescence spectra of **3aa** and **3ga** in CH_3OH.

3.3 Photophysical Properties of 3aa and 3ga.

Table S2. Photophysical properties of **3aa** and **3ga** in CH_3OH.

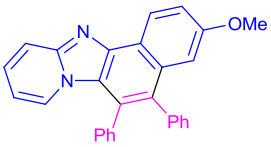
Compound	λ_{abs} (nm)	λ_{em} (nm)	Stoke's shift (nm)
3aa	202, 256, 280, 303 318, 333, 363	423	60
3ga	204, 262, 285, 309 336, 349, 379	419	40

4 References

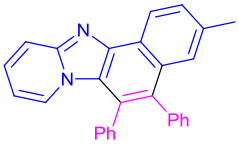
[1] Y. Li, B.-J. Li, W.-H. Wang, W.-P. Huang, X.-S. Zhang, K. Chen and Z.-J. Shi, *Angew. Chem., Int. Ed.*, 2011, **50**, 2115.

[2] W. Zhang, S. Lou, Y. Liu and Z. Xu, *J. Org. Chem.*, 2013, **78**, 5932.

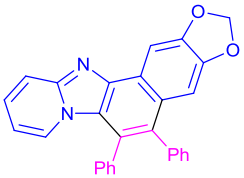
5 Characterization data for the products



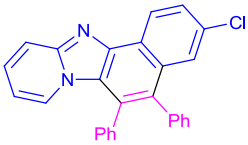
(**3ba**): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (60.0 mg, 75% yield) as a yellow solid. Mp. 258-259 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.88 (d, J = 8.9 Hz, 2H), 7.81 (d, J = 9.1 Hz, 1H), 7.37-7.18 (m, 13H), 6.96 (s, 1H), 6.48 (t, J = 6.8 Hz, 1H), 3.71 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.00, 148.01, 141.01, 138.60, 136.96, 132.85, 132.65, 131.46, 130.26, 128.42, 127.62, 127.57, 127.10, 127.06, 126.57, 126.57, 126.35, 124.50, 120.77, 117.51, 116.87, 110.42, 108.00, 55.11. MS (EI): 400 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{28}H_{21}N_2O$ $(M+H)^+$ 401.1648, found 401.1646. IR (KBr) v 3038, 1639, 1489, 1423 cm^{-1}.



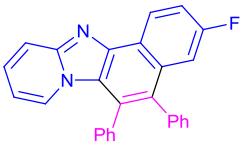
(**3ca**): Flash column chromatography on a silica gel (ethyl acetate: dichloromethan 1: 20) give the product (61.4 mg, 80% yield) as a yellow solid. Mp. 257-258 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.89 (s, 1H), 7.83 (d, J = 7.0 Hz, 1H), 7.54 (s, 1H), 7.38 (s, 1H), 7.31-7.17 (m, 12H), 6.48 (t, J = 6.8, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.63, 137.00, 135.89, 134.48, 133.14, 131.57 (d), 130.34 (d), 128.40, 128.16 (d), 127.45, 127.11, 126.80, 126.63, 126.48, 124.43, 124.01, 122.79, 117.68, 110.52 (d), 22.02. MS (EI): 384 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{28}H_{21}N_2$ $(M+H)^+$ 385.1699, found 385.1698. IR (KBr) v 3053, 1627, 1491, 1441, 1352 cm^{-1}.



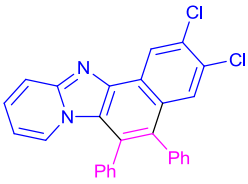
(**3da**): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (57.1 mg, 69% yield) as a greenish solid. Mp. 241-242 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.59 (d, J = 8.3 Hz, 1H), 7.80 (d, J = 8.8 Hz, 1H), 7.38-7.14 (m, 13H), 6.49 (t, J = 6.5 Hz, 1H), 5.77 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.34, 142.93, 139.35, 136.45, 131.08, 130.40 (d), 129.15, 128.40, 127.83, 127.68, 127.21, 126.52 (d), 126.33 (d), 126.20, 122.38, 117.86, 117.57, 117.07, 110.71, 110.09, 100.66. MS (EI): 414 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{28}H_{19}N_2O_2$ $(M+H)^+$ 415.1441, found 415.1441. IR (KBr) v 2924, 1636, 1497, 1431, 1352 cm^{-1}.



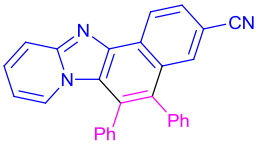
(3ea): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (50.1 mg, 62% yield) as a yellow solid. Mp. 299-301 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.91 (s, 1H), 7.84 (d, J = 7.7 Hz, 1H), 7.66 (s, 1H), 7.58 (s, 1H), 7.33-7.16 (m, 12H), 6.53 (t, J = 6.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.79, 136.55, 132.66, 132.40, 132.19, 131.49(d), 130.18 (d), 128.57 (d), 127.95, 127.93, 127.88, 127.72, 127.61, 126.90 (d), 126.83, 126.55, 124.59, 117.85, 110.85. MS (EI): 404 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{27}H_{18}ClN_2$ $(M+H)^+$ 405.1153, found 405.1152. IR (KBr) v 2922, 1636, 1489, 1433 cm^{-1}.



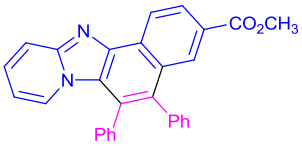
(3fa): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (54.3 mg, 70% yield) as a yellow solid. Mp. 238-240 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.97 (s, 1H), 7.82 (s, 1H), 7.45 (s, 1H), 7.34-7.16 (m, 13H), 6.50 (t, J = 6.8, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.4 (d, $J_{C\text{-}F}$ = 242.6 Hz)， 138.0, 136.6, 132.8 (d, $J_{C\text{-}F}$ = 5.12 Hz), 131.4 (d), 130.2 (d), 128.5 (d), 127.8, 128.7 (d), 127.4, 127.3, 126.8, 126.5 (d, $J_{C\text{-}F}$ = 1.7 Hz), 125.2 (d, $J_{C\text{-}F}$ = 8.5 Hz), 122.8, 117.8, 115.65 (d, $J_{C\text{-}F}$ = 24.5 Hz), 111.7 (d, $J_{C\text{-}F}$ = 22.4 Hz), 110.7. MS (EI): 388 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{27}H_{18}FN_2$ $(M+H)^+$ 389.1449, found 389.1447. IR (KBr) v 3055, 1628, 1491, 1439, 1350 cm^{-1}.



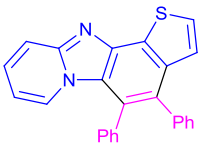
(3ga): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (58.7 mg, 67% yield) as a yellow solid. Mp. 323-325 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.04 (s, 1H), 7.84 (d, J = 9.1 Hz, 1H), 7.67 (s, 1H), 7.36-7.33 (m, 4H), 7.30-7.22 (m, 6H), 7.17-7.15 (m, 2H), 6.54 (t, J = 6.7, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.37, 139.74, 137.45, 136.25, 132.34, 131.42, 130.68, 130.64, 130.40 (d), 130.13, 128.77, 128.63(d), 128.01, 127.90, 127.80, 126.48, 125.10, 124.34, 123.21, 117.91, 111.09. MS (EI): 438 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{27}H_{17}Cl_2N_2$ $(M+H)^+$ 439.0763, found 439.0762. IR (KBr) v 3053, 1637, 1491, 1431, 1352, 1265, 1119 cm^{-1}.



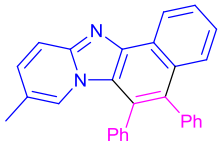
(3ha): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (49.8 mg, 63% yield) as a yellow solid. Mp. 269-270 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.00 (d, J = 8.4 Hz, 1H), 7.99 (t, J = 8.3, 1H), 7.86-7.79 (m, 2H), 7.38-7.15 (m, 12H), 6.56 (t, J = 6.9, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.50, 136.99, 135.91, 133.38, 133.26, 132.38, 131.32, 130.56, 129.96, 128.65, 128.47, 128.15, 128.10, 127.83, 127.76, 127.22, 126.82, 126.48, 126.18, 124.03, 119.59, 117.95, 112.23, 109.19. MS (EI): 395 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{28}H_{18}N_3$ $(M+H)^+$ 396.1495, found 396.1492. IR (KBr) ν 3055, 2222, 1637, 1502, 1489, 1441, 1356 cm^{-1}.



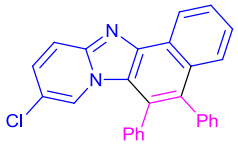
(3ia): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (62.5 mg, 73% yield) as a yellow solid. Mp. 229-230 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.02 (d, J = 8.5 Hz, 1H), 8.40 (s, 1H), 8.31 (t, J = 8.4 Hz, 1H), 8.12-8.00 (m, 1H), 7.92-7.85 (m, 1H), 7.34-7.26 (m, 9H), 7.20 (d, J = 7.4 Hz, 2H), 6.54 (t, J = 6.9 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.41, 140.41, 137.71, 136.50, 134.47, 131.53, 130.71, 130.33, 130.25, 130.07, 128.58, 127.90, 127.66, 127.60, 127.53, 126.93, 126.54, 125.89, 125.74, 123.21, 118.00, 117.72, 112.76, 110.97, 52.13. MS (EI): 428 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{29}H_{21}N_2O_2$ $(M+H)^+$ 429.1598, found 429.1595. IR (KBr) ν 2950, 2928, 1711, 1637, 1504, 1433, 1356 cm^{-1}.



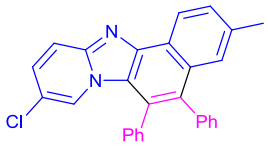
(3ja): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (56.4 mg, 75% yield) as a orange solid. Mp. 237-238 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.80-7.78 (m, 1H), 7.48-7.47 (m, 1H), 7.35-7.16 (m, 13H), 6.49 (t, J = 6.8, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.00, 138.16, 136.46, 130.98 (d), 130.75 (d), 128.87, 128.52, 128.11, 127.79 (d), 127.52 (d), 126.99, 126.56, 125.37, 125.29, 124.33, 117.75, 110.36. MS (EI): 376 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{25}H_{17}N_2S$ $(M+H)^+$ 377.1107, found 377.1105. IR (KBr) ν 3043, 1637, 1501, 1413, 1348 cm^{-1}.



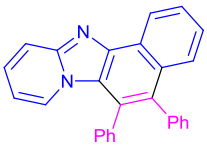
(3ka): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (62.2 mg, 81% yield) as a yellow solid. Mp. 285-286 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.95 (d, J = 8.1, 1H), 7.74-7.72 (m, 1H), 7.68 (t, J = 7.4 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.48 (t, J = 7.6 Hz, 1H), 7.25-7.13 (m, 11H), 6.95 (s, 1H), 2.02 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.11, 140.83, 138.63, 137.00, 133.07, 131.57, 131.26, 130.36, 130.31, 128.34, 127.54, 127.51, 127.46, 126.66, 126.51, 126.09, 126.03, 125.95, 124.17, 122.81, 122.49, 119.85, 116.99, 18.39. MS (EI): 384 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{28}H_{21}N_2$ $(M+H)^+$ 385.1699, found 395.1698. IR (KBr) v 3026, 1647, 1572, 1492, 1408 cm^{-1}.



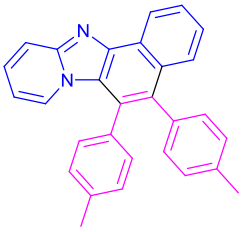
(3la): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (63.0 mg, 78% yield) as a yellow solid. Mp. 210-211 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.94 (t, J = 8.0 Hz, 1H), 8.09 (s, 1H), 7.90 (d, J = 7.5 Hz, 2H), 7.78-7.70 (m, 2H), 7.62 (d, J = 8.3 Hz, 1H), 7.56-7.49 (m, 2H), 7.43 (t, J = 7.3 Hz, 1H), 7.37-7.33 (m, 3H), 7.28-7.24 (m, 3H), 7.19-7.17 (m, 1H), 7.11-7.09 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.05, 138.23, 136.19, 134.21, 131.43, 130.18, 128.72, 128.64, 128.33, 128.21, 127.97, 127.67, 127.55, 126.71, 126.44, 125.97, 124.37, 123.31, 122.86, 120.44, 118.43, 117.99, 117.75. MS (EI): 404 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{27}H_{18}ClN_2$ $(M+H)^+$ 405.1153, found 405.1151. IR (KBr) v 3024, 1568, 1520, 1493, 1408 , 1321 cm^{-1}.



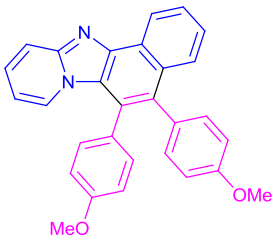
(3ma): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (63.5 mg, 76% yield) as a yellow solid. Mp. 255-256 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.83 (d, J = 8.2 Hz, 1H), 7.80-7.74 (m, 1H), 7.56 (d, J = 8.2 Hz, 1H), 7.38-7.36 (m, 3H), 7.29-7.24 (m, 10H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.07, 138.38, 136.35, 136.30, 133.86, 131.74, 131.49, 130.22, 129.44, 128.63, 128.45, 128.22, 127.92, 127.56, 126.95, 126.66, 126.39, 124.36, 124.00, 122.80, 122.33, 118.33, 117.94, 22.06. MS (EI): 418 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{28}H_{20}ClN_2$ $(M+H)^+$ 419.1310, found 419.1307. IR (KBr) v 3051, 2359, 1601, 1491, 1418, 1323 cm^{-1}.



(3aa): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (61.4 mg, 83% yield) as a yellow solid. Mp. 237-238 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.98 (d, J = 7.2 Hz, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.71 (s, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.51 (d, J = 6.8 Hz, 1H), 7.26 (m, 12H), 6.49 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.01, 140.88, 140.44, 138.57, 136.91, 131.57, 131.43, 130.36, 128.47, 127.69, 127.57, 127.49, 127.18, 126.59, 126.57, 126.45, 126.16, 126.15, 126.01, 122.94, 122.62, 117.83, 110.58. MS (EI): 371 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{27}H_{19}N_2$ $(M+H)^+$ 371.1543, found 371.1542. IR (KBr) v 3055, 1626, 1493, 1423, 1352 cm^{-1}.

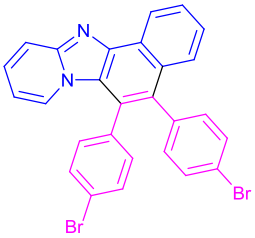


(3ab): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (63.7 mg, 80% yield) as a yellow solid. Mp. 249-250 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.96 (d, J = 8.1 Hz, 1H), 7.85 (d, J = 9.1 Hz, 1H), 7.69 (t, J = 7.4 Hz, 1H), 7.61 (d, J = 8.5 Hz, 1H), 7.50-7.41 (m, 1H), 7.31 (t, J = 7.3 Hz, 2H), 7.14 (s, 4H), 7.07 (s, 4H), 6.51 (t, J = 6.9 Hz, 1H), 2.38 (s, 3H), 2.33 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 147.86, 140.57, 137.21, 135.92, 135.55, 133.84, 133.67, 131.70, 131.36, 130.11, 129.22, 128.69, 128.24, 127.62, 127.18, 126.66, 126.58, 126.04, 126.00, 125.91, 122.88, 117.69, 110.54, 21.37, 21.24. MS (EI): 398 (M+); HRMS (ESI-TOF) m/z calcd for $C_{29}H_{23}N_2$ $(M+H)^+$ 399.1856, found 399.1856. IR (KBr) v 3051, 2920, 1634, 1506, 1421, 1358 cm^{-1}.

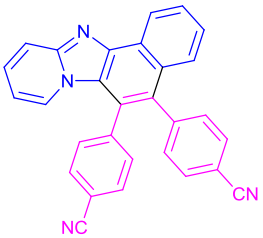


(3ac): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (66.2 mg, 77% yield) as a yellow solid. Mp. 248-250 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.96 (d, J = 8.0, 1H), 7.85 (d, J = 8.2 Hz, 1H), 7.69 (t, J = 7.1 Hz, 1H), 7.64 (d, J = 8.3, 1H), 7.50 (t, J = 7.3 Hz, 1H), 7.38 (d, J = 7.0 Hz, 1H), 7.34-7.30 (m, 1H), 7.15 (d, J = 8.6 Hz, 2H), 7.10 (d, J = 8.5 Hz, 2H), 6.88 (d, J = 8.6 Hz, 2H), 6.81 (d, J = 8.5 Hz, 2H), 6.53 (t, J = 6.6 Hz, 1H) 3.85 (s, 1H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.80, 158.08, 147.93, 140.71, 133.67, 132.54, 131.88, 131.41, 130.96, 129.24, 129.19, 127.60, 127.17, 126.60, 126.57, 126.08, 126.02, 122.93, 117.79, 116.30, 113.93, 113.03, 110.59, 55.18,

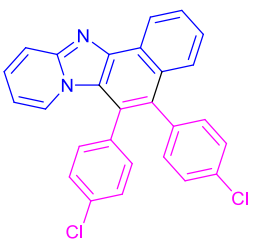
55.13. MS (EI): 430 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{29}H_{23}N_2O_2$ $(M+H)^+$ 431.1754, found 431.1752. IR (KBr) *v* 3031, 1609, 1506, 1456, 1421, 1354, 1288 cm^{-1}.



(3ad): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (46.2 mg, 44% yield) as a yellow solid. Mp. 294-295 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.96 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 9.0 Hz, 1H), 7.74-7.70 (m, 1H) 7.55-7.48 (m, 4H), 7.46-7.41 (m, 2H), 7.37-7.34 (m, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 2H), 6.59 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.12, 141.15, 137.28, 135.56, 133.09, 132.94, 132.16, 131.95, 131.90, 131.63, 130.98, 127.52, 127.22, 126.54, 126.46, 126.13, 125.25, 123.04, 122.24, 122.11, 121.10, 117.99, 111.04. MS (EI): 525 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{27}H_{17}Br_2N_2$ $(M+H)^+$ 526.9753, found 526.9751. IR (KBr) *v* 3055, 1622, 1491, 1467, 1352, 1275 cm^{-1}.

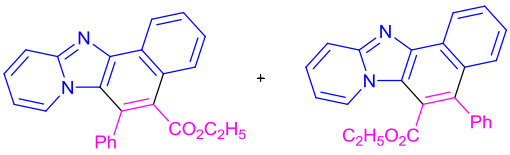


(3ae): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (43.7 mg, 52% yield) as a yellow solid. Mp. 167-168 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.00 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 9.1 Hz, 1H), 7.78 (d, *J* = 7.3 Hz, 1H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.61-7.54 (m, 3H), 7.46-7.38 (m, 4H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 7.1 Hz, 1H), 6.63 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 148.37, 143.30, 141.65, 141.37, 132.52, 132.26, 131.69, 131.28, 131.18, 130.31, 127.93, 127.11, 126.94, 126.83, 126.38, 125.69, 124.57, 123.29, 121.45, 118.50, 118.29, 118.06, 112.44, 111.49, 111.24. MS (EI): 420 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{29}H_{17}N_4$ $(M+H)^+$ 421.1448, found 421.1446. IR (KBr) *v* 3360, 2922, 2230, 1637, 1502, 1425, 1354 cm^{-1}.



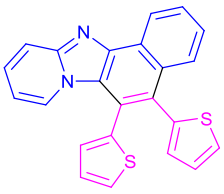
(3af): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (56.1 mg, 64% yield) as a yellow solid. Mp. 233-235 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.97 (d, *J* = 8.2 Hz, 1H), 7.87-7.85 (m, 1H), 7.74-7.70 (m, 1H), 7.56-7.50 (m, 2H),

7.37-7.33 (m, 4H), 7.28-7.26 (m, 2H), 7.20-7.18 (m, 2H),7.12 (d, *J* = 8.3 Hz, 2H), 6.59 (t, *J* = 6.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.16, 136.85, 135.17, 134.03, 132.88, 132.77, 131.65, 131.13, 129.01(d), 128.04, 127.48, 127.25, 126.54, 126.54, 126.46, 126.22, 126.16, 125.39, 123.08, 122.23, 118.04, 110.99. MS (EI): 438 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{27}H_{17}Cl_2N_2^+$ $(M+H)^+$ 439.0763, found 439.0760. IR (KBr) *v* 3061, 1636, 1493, 1425, 1354, 1261, 1092 cm^{-1}.



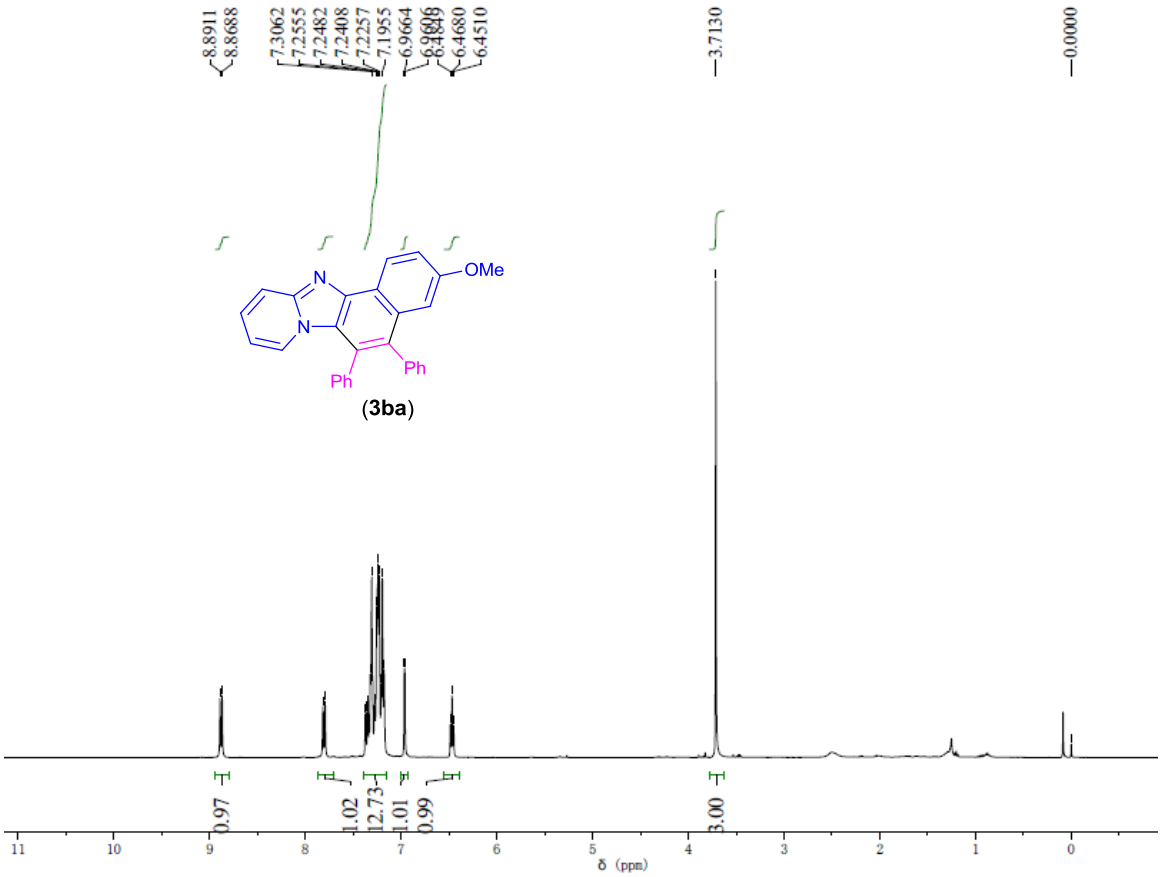
3ag 3ag'

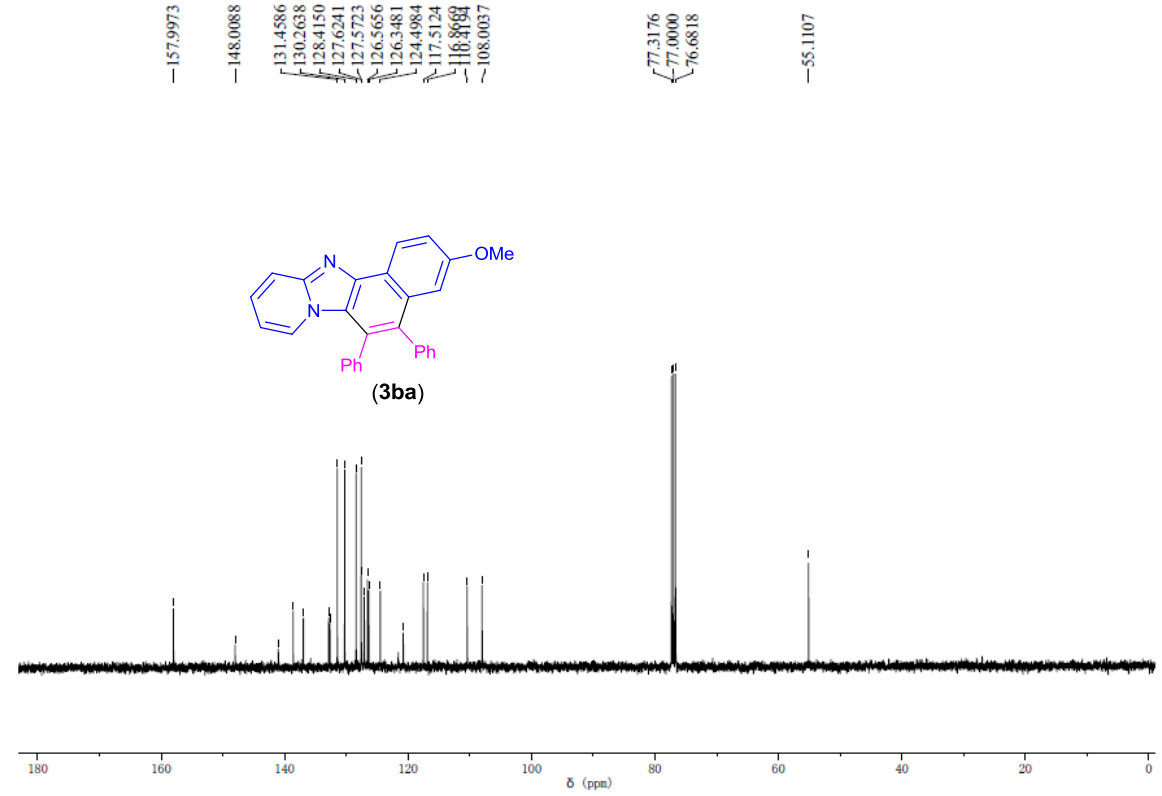
(3ag + 3ag'): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 15) give the product (**3ag + 3ag' =** 58.6 mg, 80% yield) as a yellow solid. Mp. 168-170 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.94 (s, 2H), 8.54 (d, *J* = 6.5 Hz, 2H), 8.08 (d, *J* = 8.2 Hz, 1H), 7.90-7.87 (m, 2H), 7.73-7.65 (m, 4H), 7.55-7.40 (m, 11H), 7.34-7.31 (m, 1H), 6.89 (t, *J* = 6.8 Hz, 1H), 6.53 (t, *J* = 6.8 Hz, 1H), 4.15-4.10 (m, 1H), 0.98 (t, *J* = 7.1 Hz, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.74, 168.04, 138.10, 135.60, 133.29, 130.69, 130.47, 129.61, 128.82, 128.76, 128.17, 128.03, 127.95, 127.76, 127.65, 127.33, 127.10, 127.06, 126.64, 126.42, 126.32, 126.28, 125.92, 125.88, 125.56, 123.17, 123.01, 117.91, 117.84, 61.76, 61.12, 13.68, 13.41. MS (EI): 366 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{24}H_{19}N_2O_2$ $(M+H)^+$ 367.1441, found 367.1441. IR (KBr) *v* 3057, 1709, 1637, 1495, 1425, 1354 cm^{-1}.

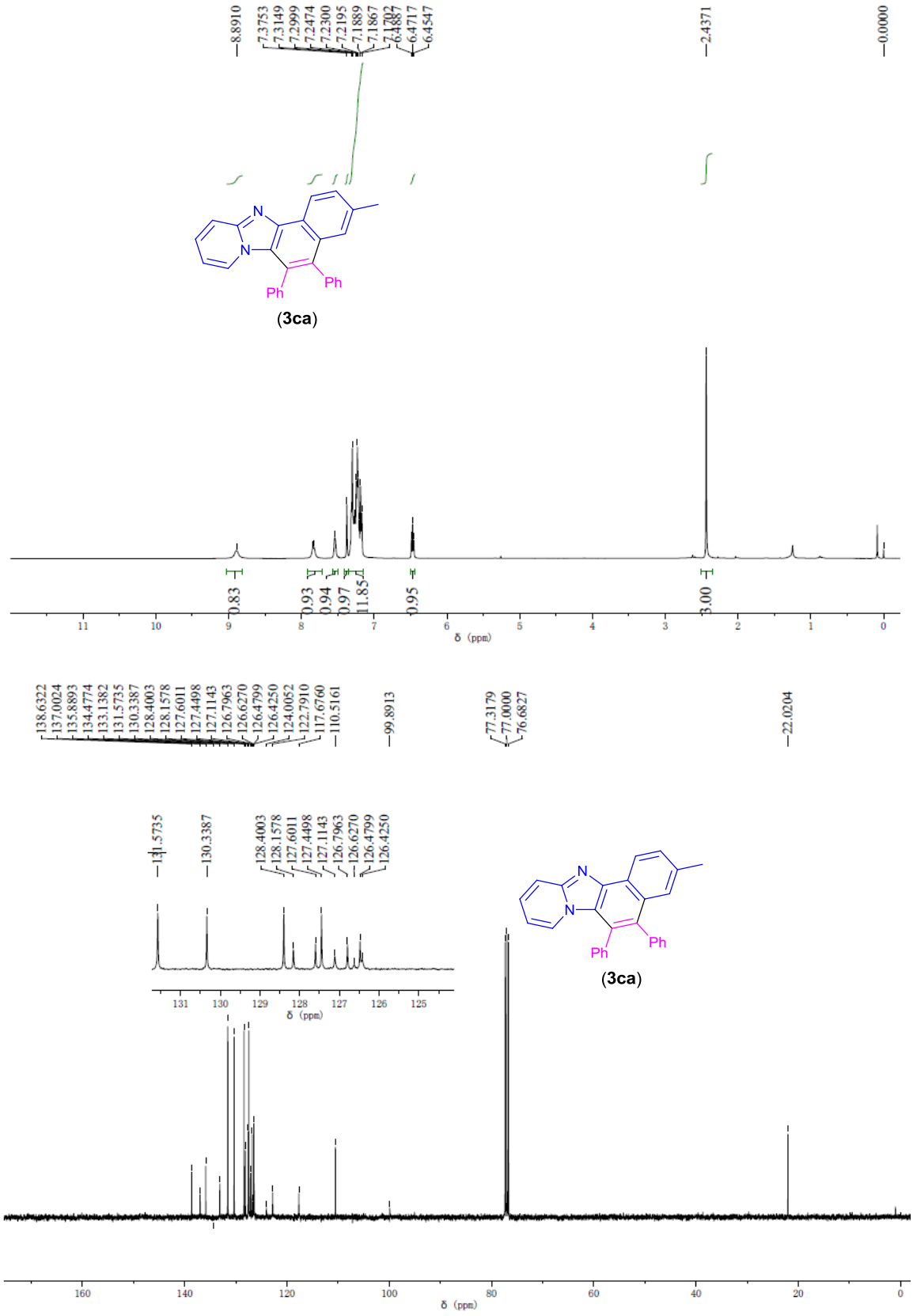


(3ah): Flash column chromatography on a silica gel (ethyl acetate: dichloromethane, 1: 20) give the product (45.8 mg, 60% yield) as a brownish solid. Mp. 224-225 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.93 (d, *J* = 8.1 Hz, 1H), 7.85 (t, *J* = 8.6 Hz, 2H), 7.73 (t, *J* = 7.3 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.45-7.35 (m, 4H), 7.12-6.98 (m, 4H), 6.63 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.33, 141.54, 138.64, 136.77, 132.10, 129.91, 129.11, 127.98, 127.77, 127.57, 127.38, 127.28, 126.86, 126.56, 126.48, 126.39, 126.32, 126.29, 123.09, 122.92, 121.01, 117.80, 111.07. MS (EI): 382 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{23}H_{15}N_2S_2$ $(M+H)^+$ 383.0671, found 383.0669. IR (KBr) *v* 3067, 2922, 1636, 1495, 1425 cm^{-1}.

6 Copies of ^{1}H NMR and ^{13}C NMR spectra



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6.4547
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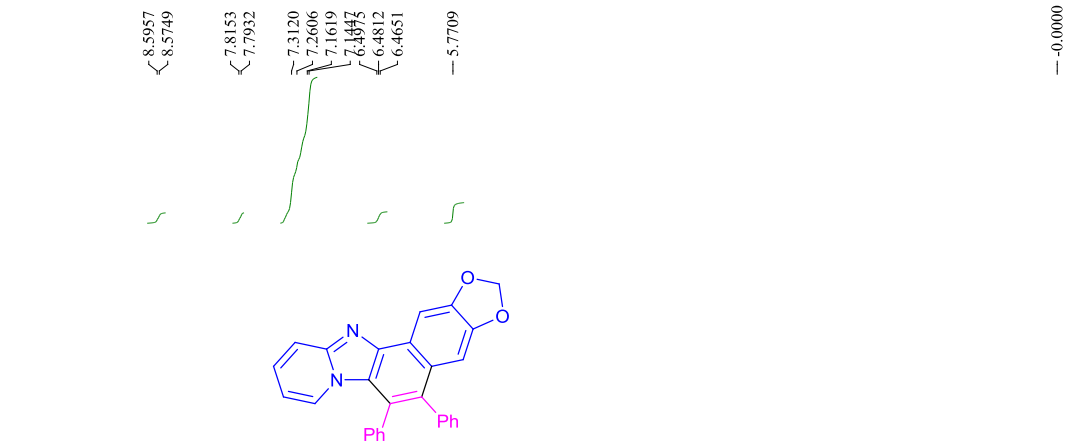
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O
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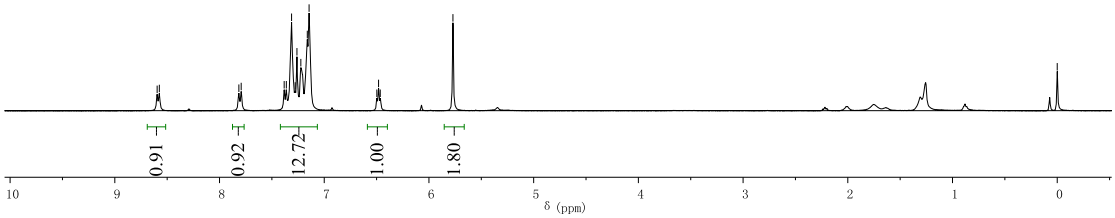
N
Ph
Ph

(**3da**)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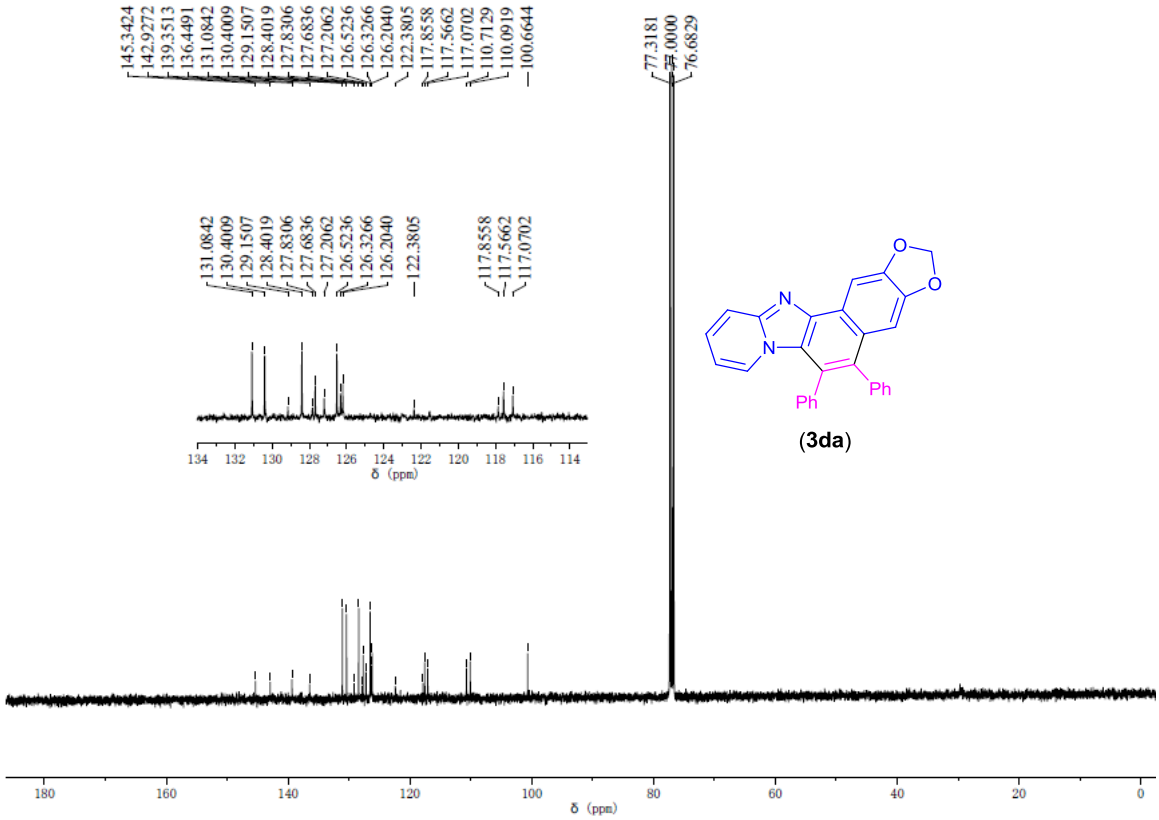
δ (ppm)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122
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118
116
114
δ (ppm)
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100
80
60
40
20
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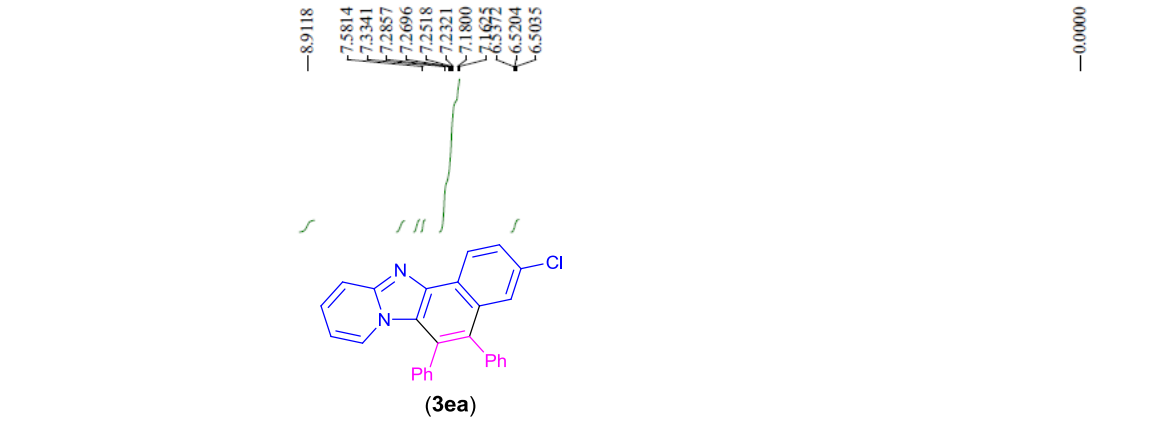
δ (ppm)

O
O
N
N
Ph
Ph

(**3da**)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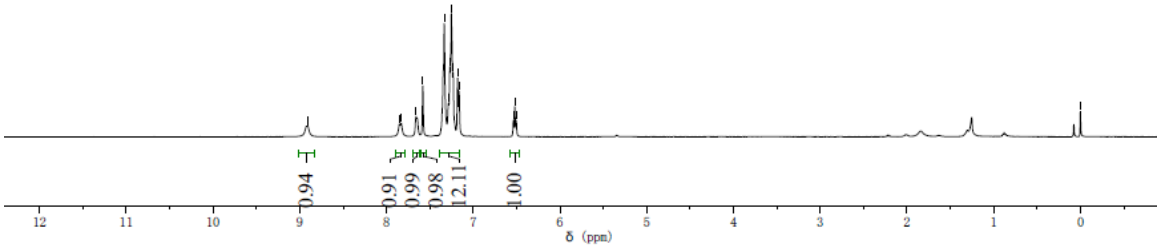
(**3ea**)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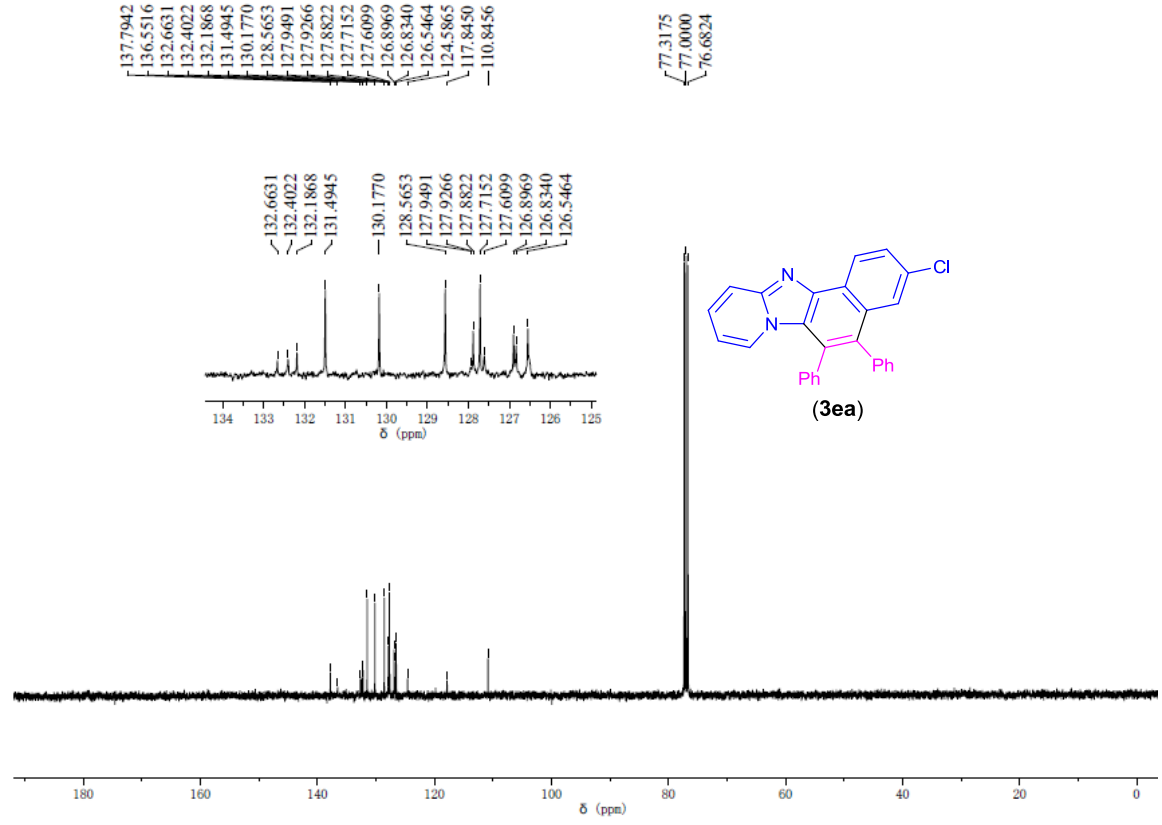
δ (ppm)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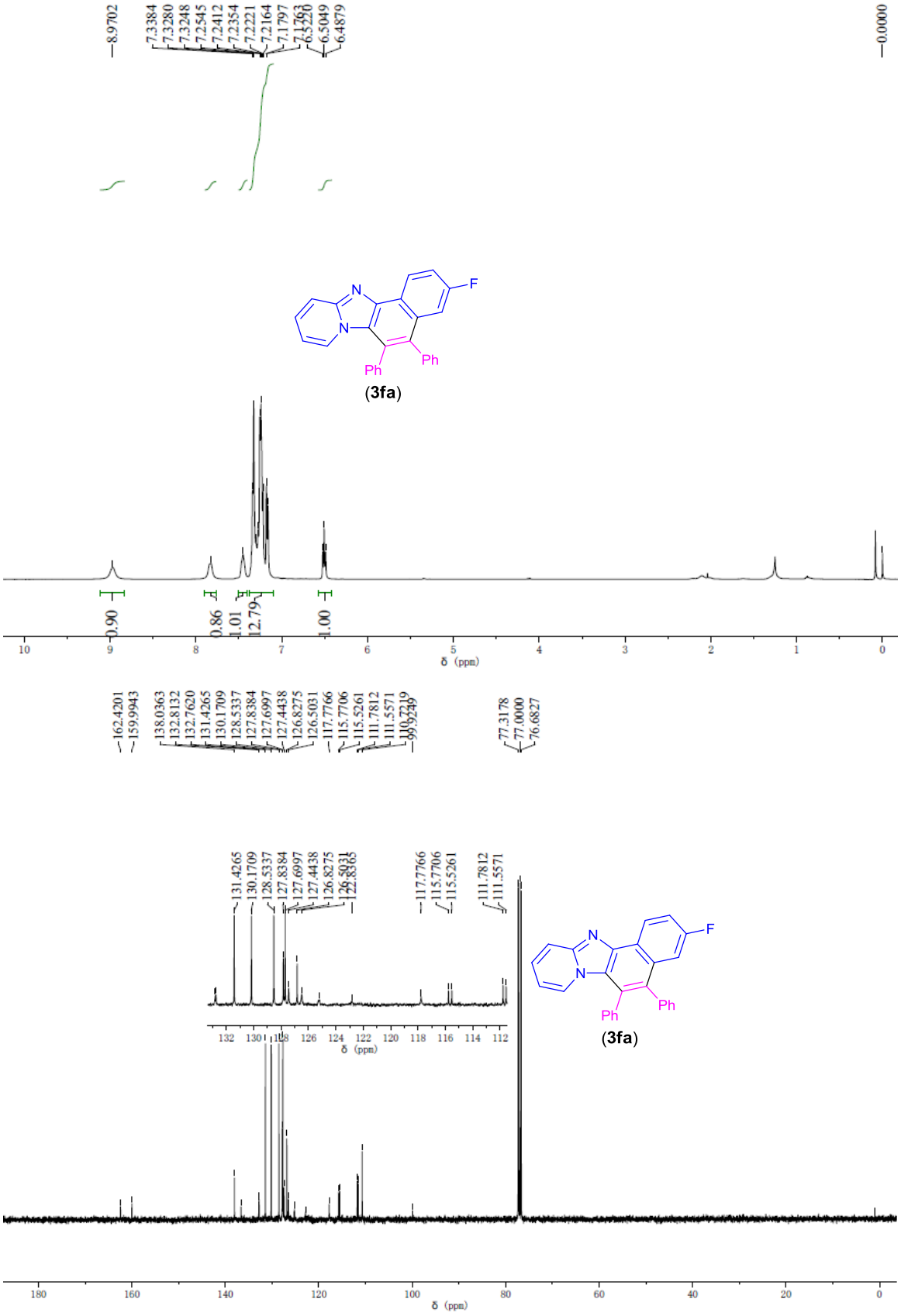
Cl
Ph
Ph

(**3ea**)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N
F
Ph
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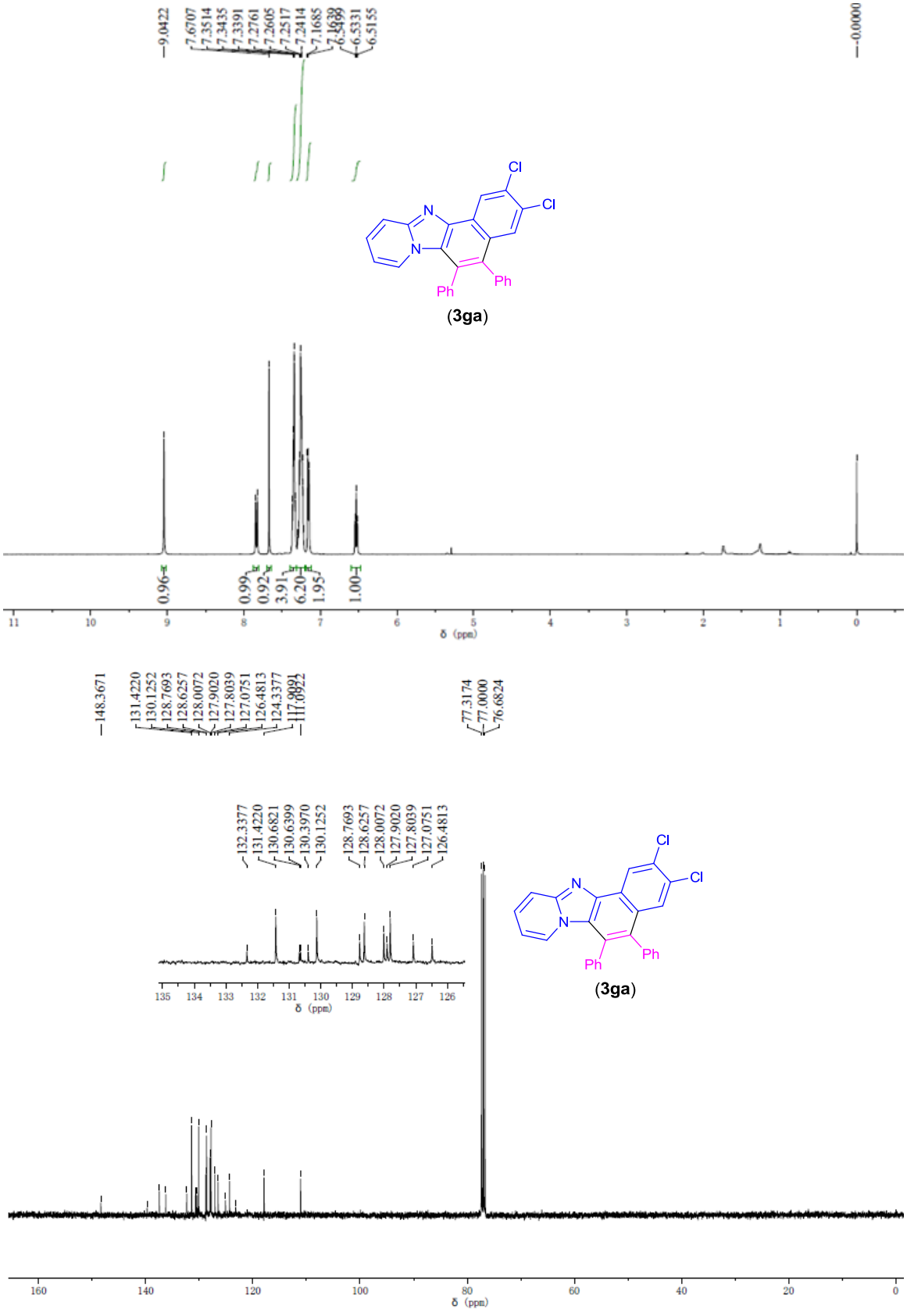
δ (ppm)
δ (ppm)

(3fa)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Cl
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N
Ph
Ph
(3ga)
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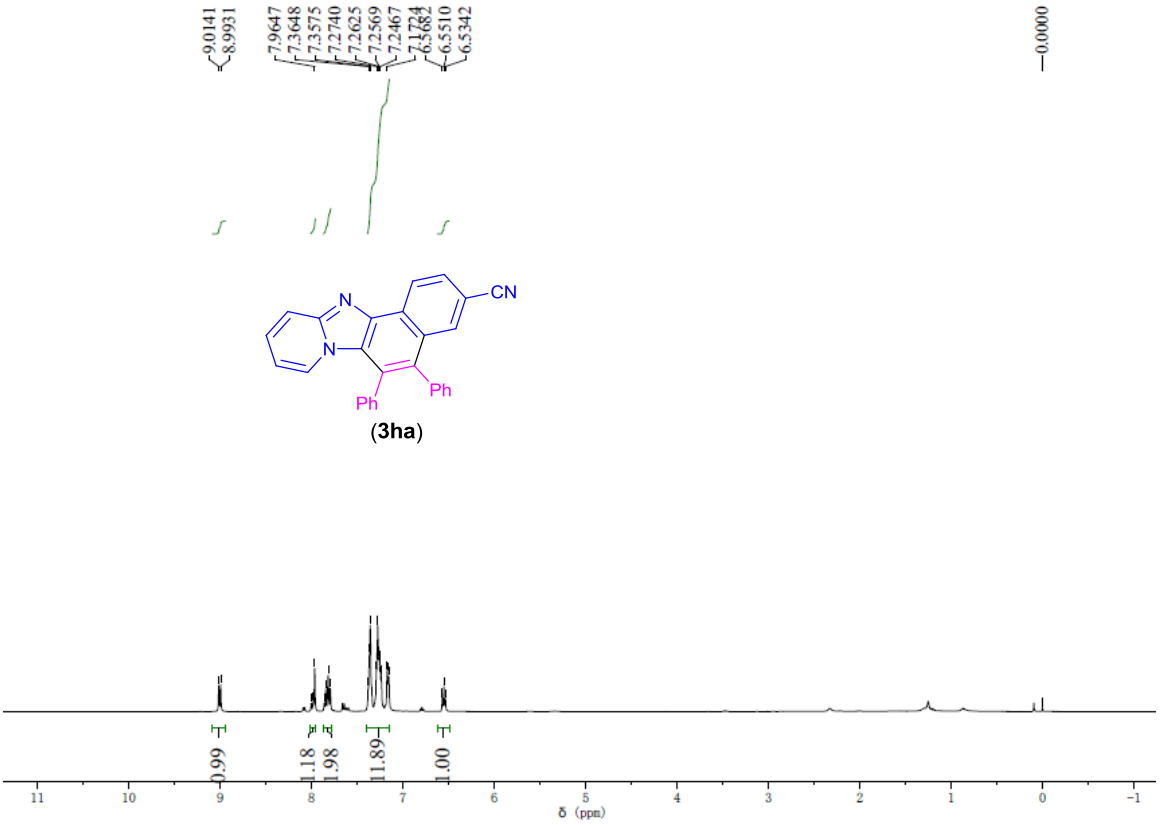
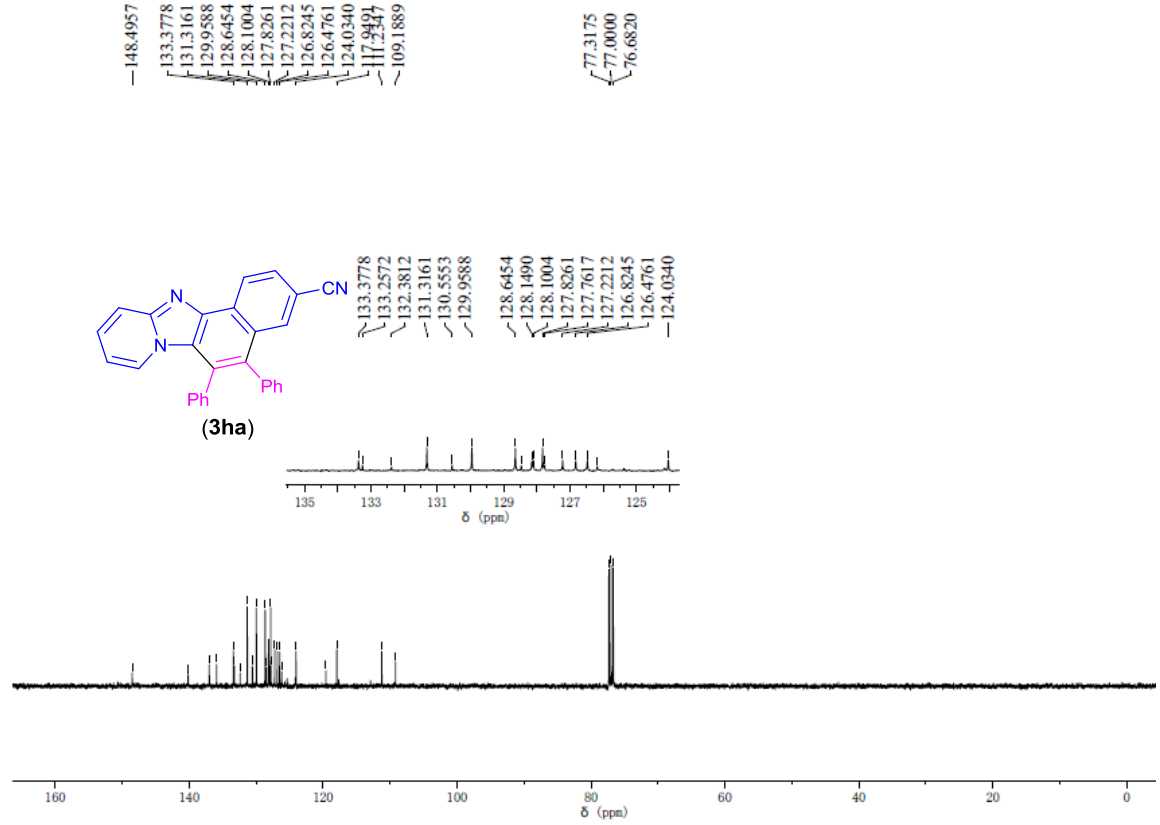
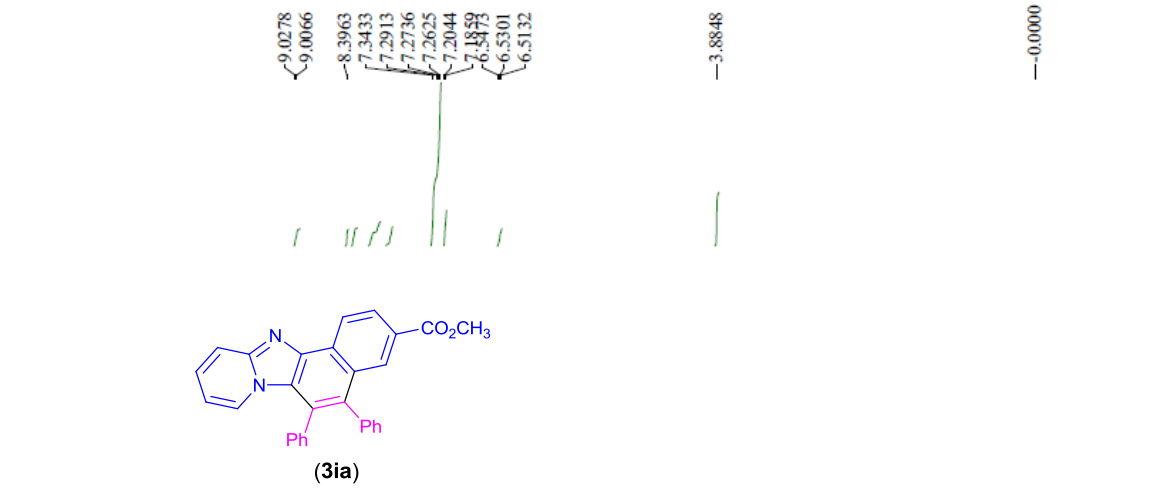
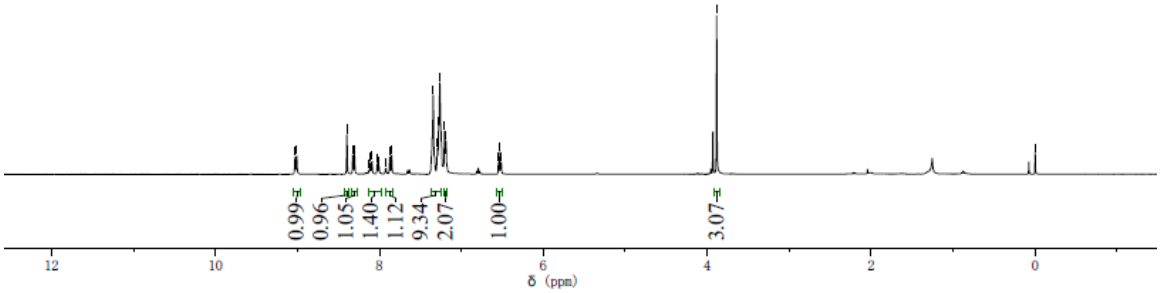
0.99
0.92
3.91
6.20
1.95
1.00
δ (ppm)
148.3671
131.4220
130.1252
128.7693
128.6257
128.0072
127.9020
127.8039
127.0751
126.4813
124.3377
77.3174
77.0000
76.6824
132.3377
131.4220
130.6821
130.6399
130.3970
130.1252
128.7693
128.6257
128.0072
127.9020
127.8039
127.0751
126.4813
δ (ppm)
(3ga)
δ (ppm)

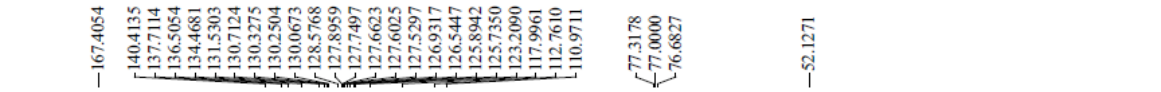

9.0141
8.9931
7.9647
7.3648
7.3575
7.2740
7.2625
7.2569
7.2467
7.1724
6.5682
6.5510
6.5342
0.0000
CN
N
N
Ph
Ph
(3ha)
0.99
1.18
1.98
11.89
1.00
δ (ppm)

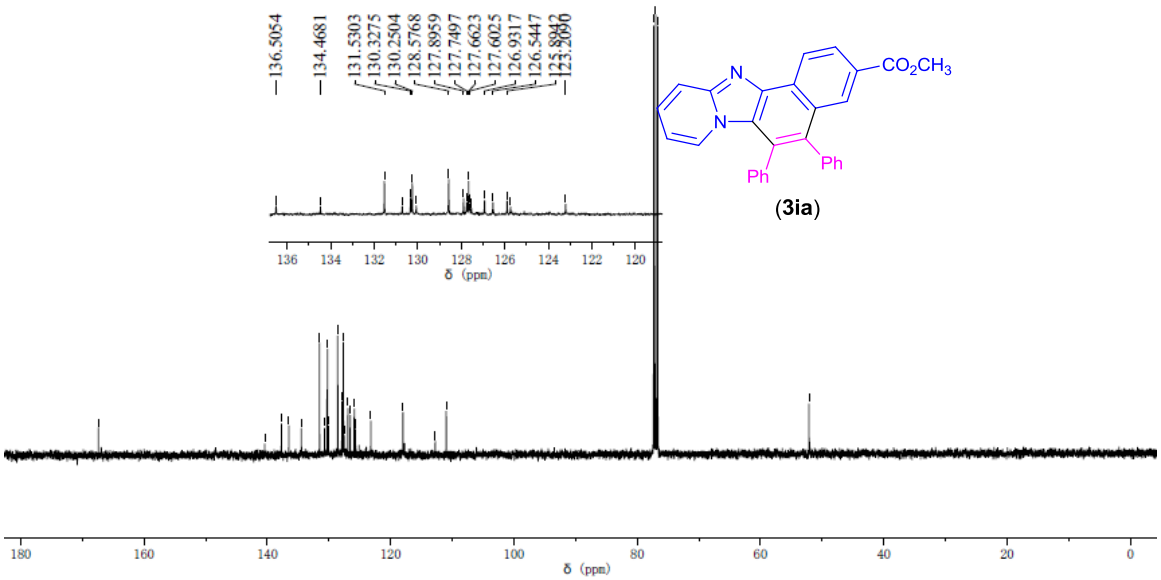

148.4957
133.3778
131.3161
129.9588
128.6454
128.1004
127.8261
127.2212
126.8245
126.4761
124.0340
109.1889
77.3175
77.0000
76.6820
CN
N
N
Ph
Ph
(3ha)
133.3778
133.2572
132.3812
131.3161
130.5553
129.9588
128.6454
128.1490
128.1004
127.8261
127.7617
127.2212
126.8245
126.4761
124.0340
δ (ppm)
δ (ppm)


9.0278
9.0066
8.3963
7.3433
7.2913
7.2736
7.2625
7.2044
7.1859
6.5473
6.5301
6.5132
3.8848
0.0000
N
N
CO2CH3
Ph
Ph

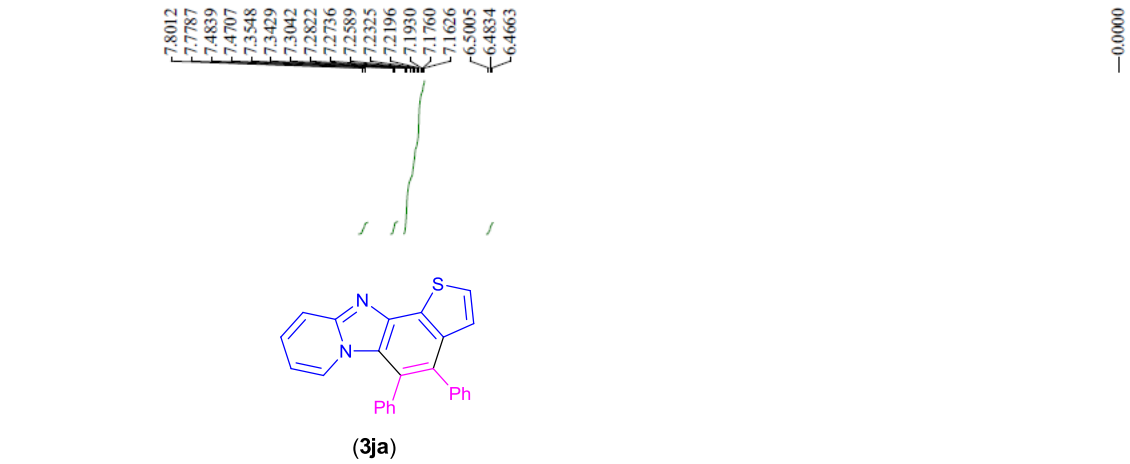
(**3ia**)


0.99
0.96
1.05
1.40
1.12
9.34
2.07
1.00
3.07
12
10
8
6
4
2
0
δ (ppm)

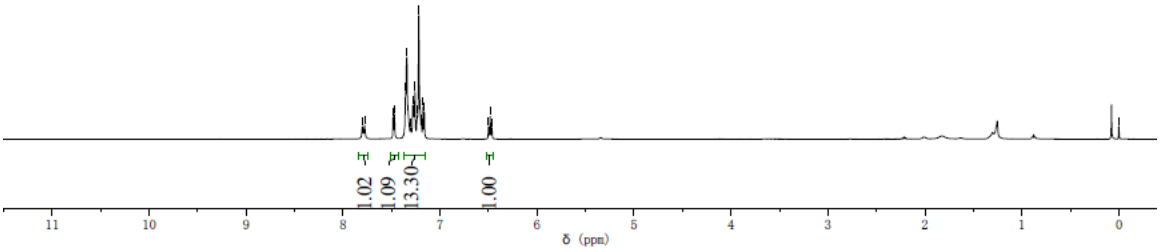

167.4054
140.4135
137.7114
136.5054
134.4681
131.5303
130.7124
130.3275
130.2504
130.0673
128.5768
127.8959
127.7497
127.6623
127.6025
127.5297
126.9317
126.5447
125.8942
125.7350
123.2090
117.9961
112.7610
110.9711
77.3178
77.0000
76.6827
52.1271

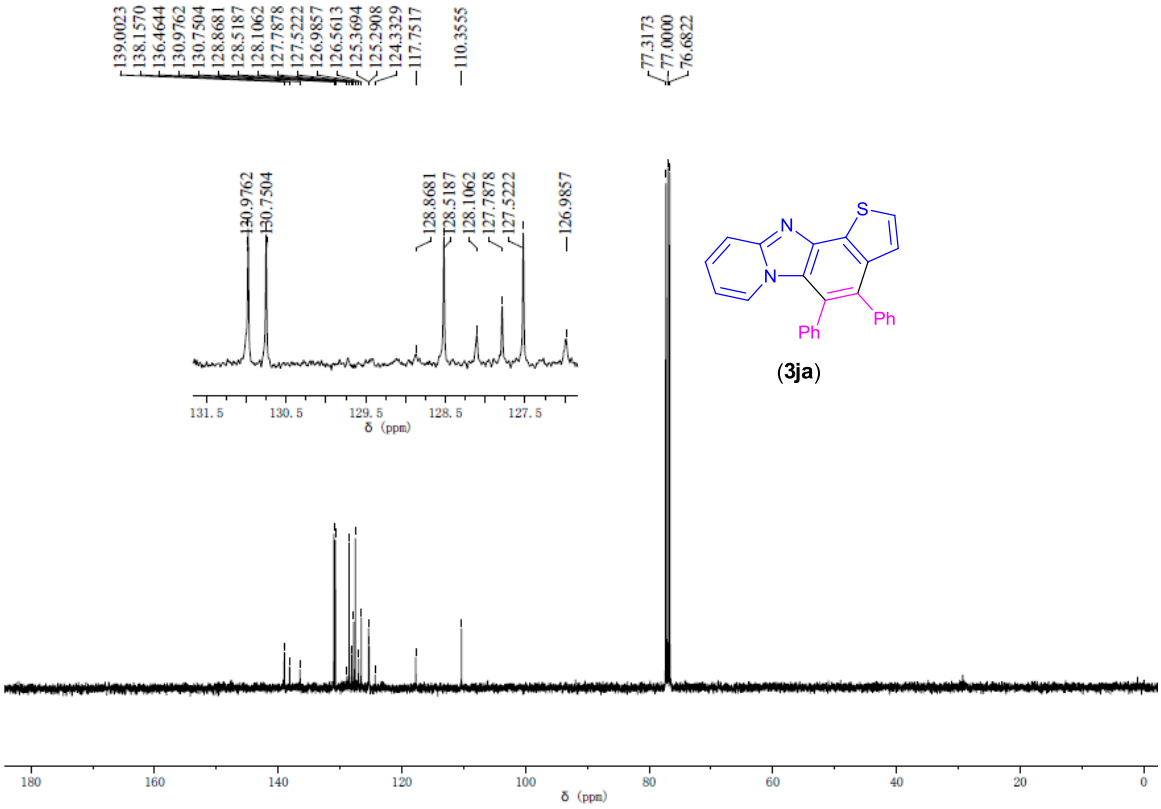

136.5054
134.4681
131.5303
130.3275
130.2504
128.5768
127.8959
127.7497
127.6623
127.6025
126.9317
126.5447
125.8942
123.2090
N
N
CO2CH3
Ph
Ph
136
134
132
130
128
126
124
122
120
δ (ppm)
180
160
140
120
100
80
60
40
20
0
δ (ppm)

(**3ia**)


7.8012
7.7787
7.4839
7.4707
7.3548
7.3429
7.3042
7.2822
7.2736
7.2589
7.2325
7.2196
7.1930
7.1760
7.1626
6.5005
6.4834
6.4663
0.0000
N
S
N
Ph
Ph

(**3ja**)

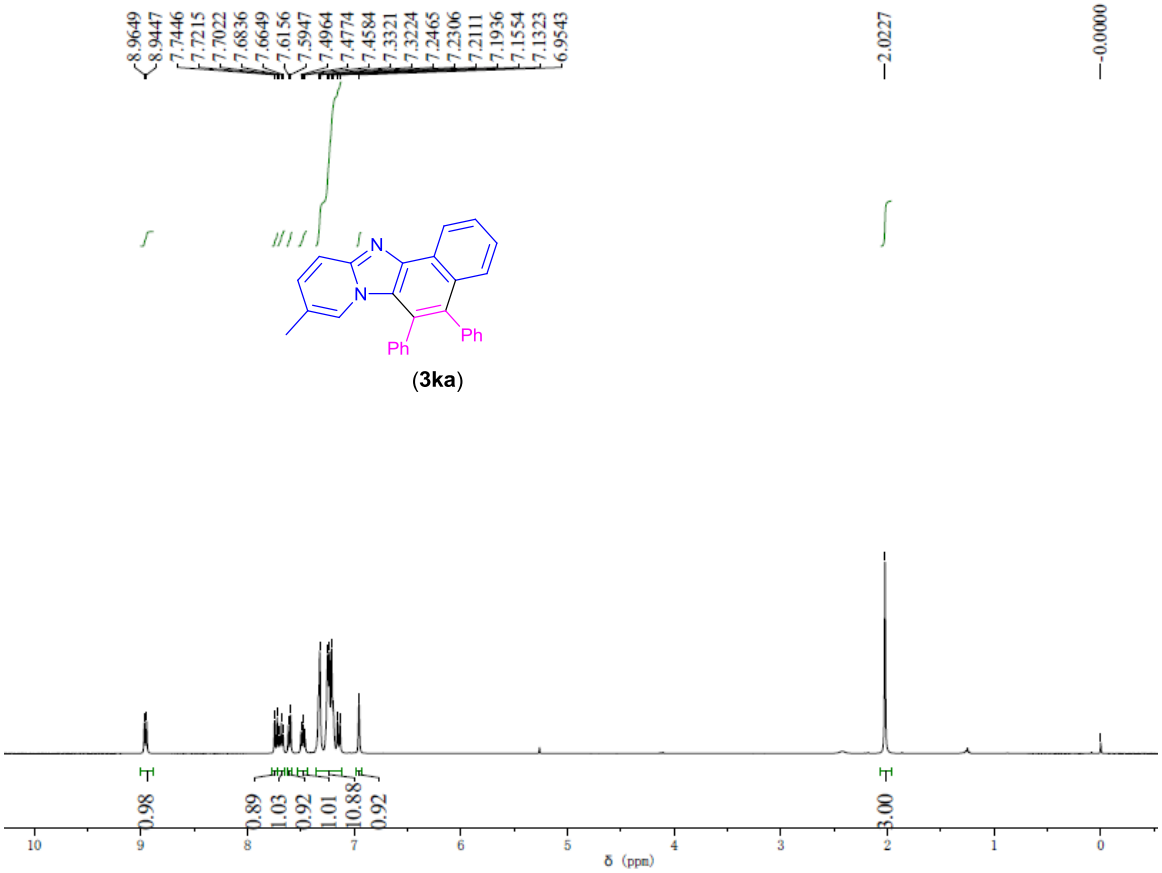

1.02
1.09
13.30
1.00
δ (ppm)


139.0023
138.1570
136.4644
130.9762
130.7504
128.8681
128.5187
128.1062
127.7878
127.5222
126.9857
126.5613
125.3694
125.2908
124.3329
117.7517
110.3555
77.3173
77.0000
76.6822
δ (ppm)

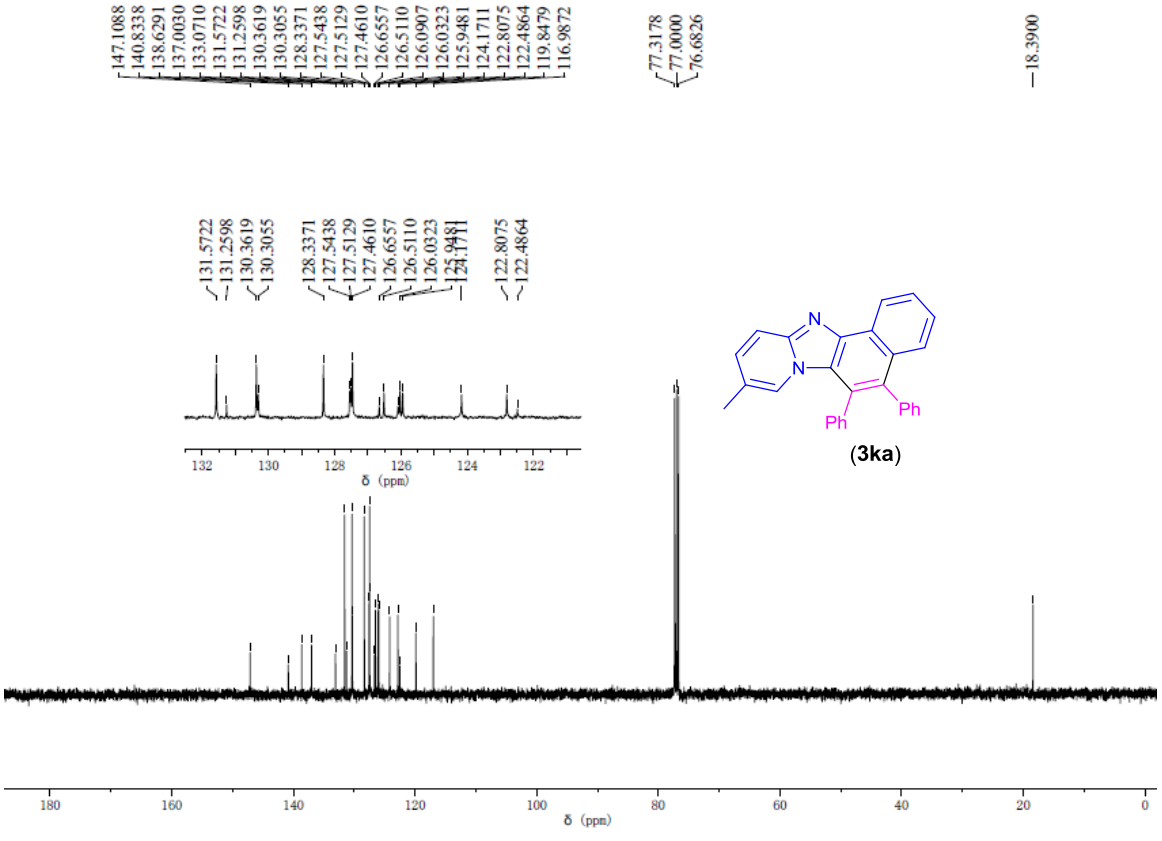
130.9762
130.7504
128.8681
128.5187
128.1062
127.7878
127.5222
126.9857
131.5
130.5
129.5
128.5
127.5
δ (ppm)

N
S
N
Ph
Ph

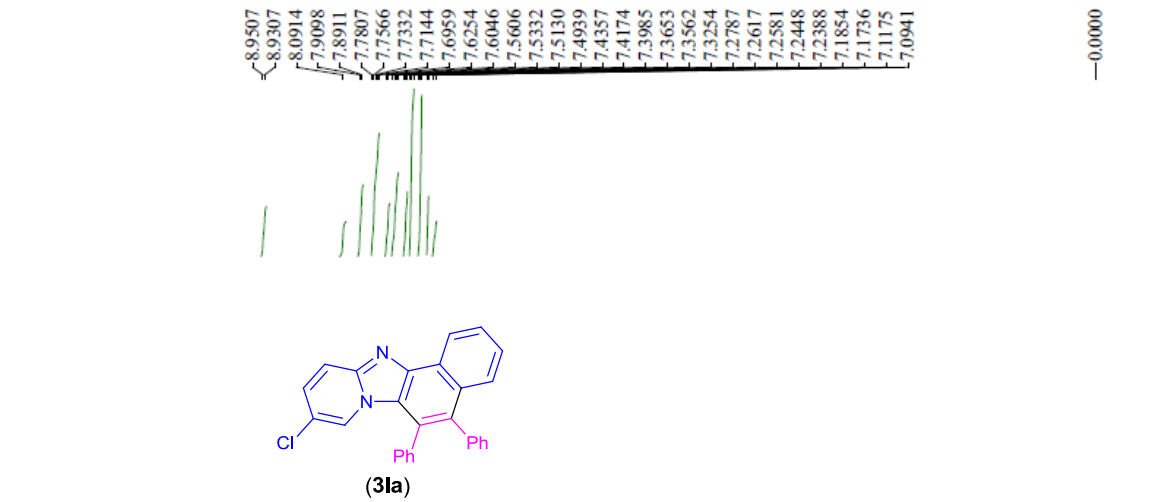
(**3ja**)


8.9649
8.9447
7.7446
7.7215
7.7022
7.6836
7.6649
7.6156
7.5947
7.4964
7.4774
7.4584
7.3321
7.3224
7.2465
7.2306
7.2111
7.1936
7.1554
7.1323
6.9543
2.0227
0.0000
N
N
Ph
Ph
0.98
0.89
1.03
0.92
1.01
10.88
0.92
3.00
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)

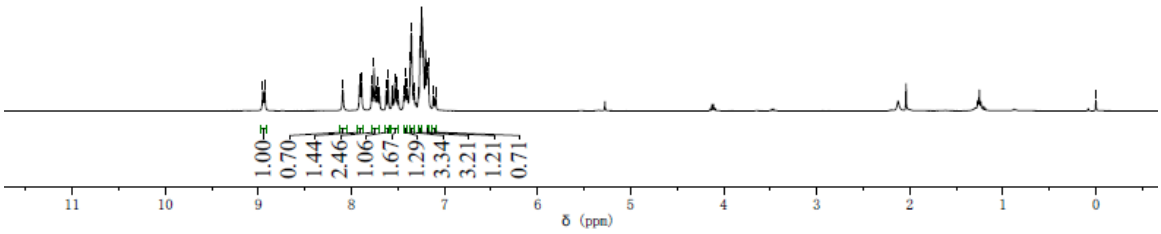
(**3ka**)

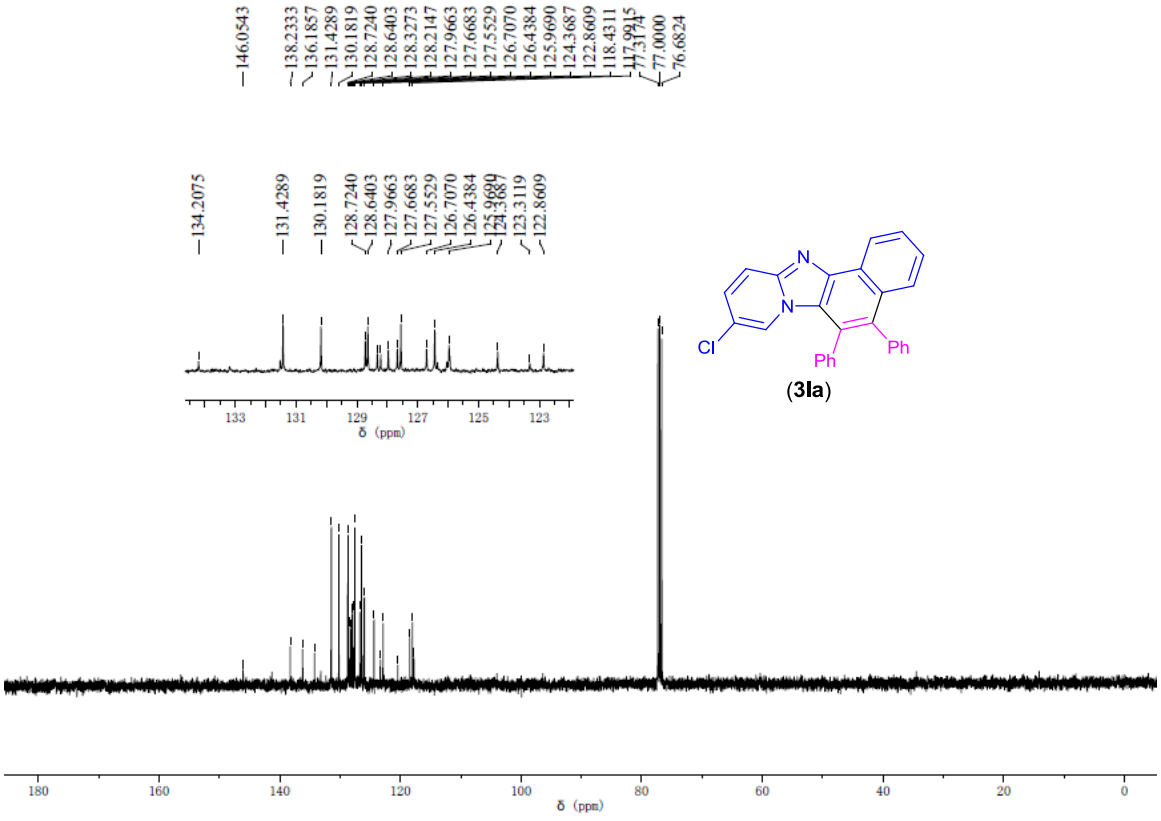

147.1088
140.8338
138.6291
137.0030
133.0710
131.5722
131.2598
130.3619
130.3055
128.3371
127.5438
127.5129
127.4610
126.6557
126.5110
126.0907
126.0323
125.9481
124.1711
122.8075
122.4864
119.8479
116.9872
77.3178
77.0000
76.6826
18.3900
131.5722
131.2598
130.3619
130.3055
128.3371
127.5438
127.5129
127.4610
126.6557
126.5110
126.0323
122.8075
122.4864
132
130
128
126
124
122
δ (ppm)
N
N
Ph
Ph
180
160
140
120
100
80
60
40
20
0
δ (ppm)

(**3ka**)

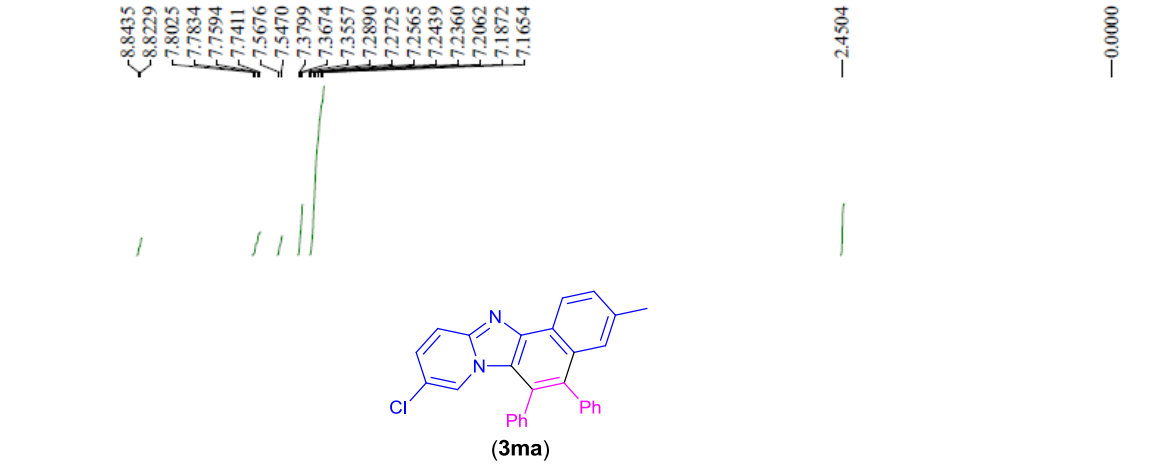

8.9507
8.9307
8.0914
7.9098
7.8911
7.7807
7.7566
7.7332
7.7144
7.6959
7.6254
7.6046
7.5606
7.5332
7.5130
7.4939
7.4357
7.4174
7.3985
7.3653
7.3562
7.3254
7.2787
7.2617
7.2581
7.2448
7.2388
7.1854
7.1736
7.1175
7.0941
0.0000
N
N
Cl
Ph
Ph

(**3la**)

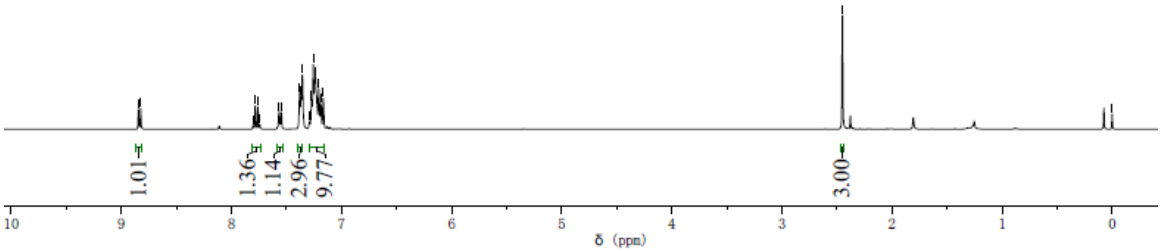

1.00
0.70
1.44
2.46
1.06
1.67
1.29
3.34
3.21
1.21
0.71
11
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)

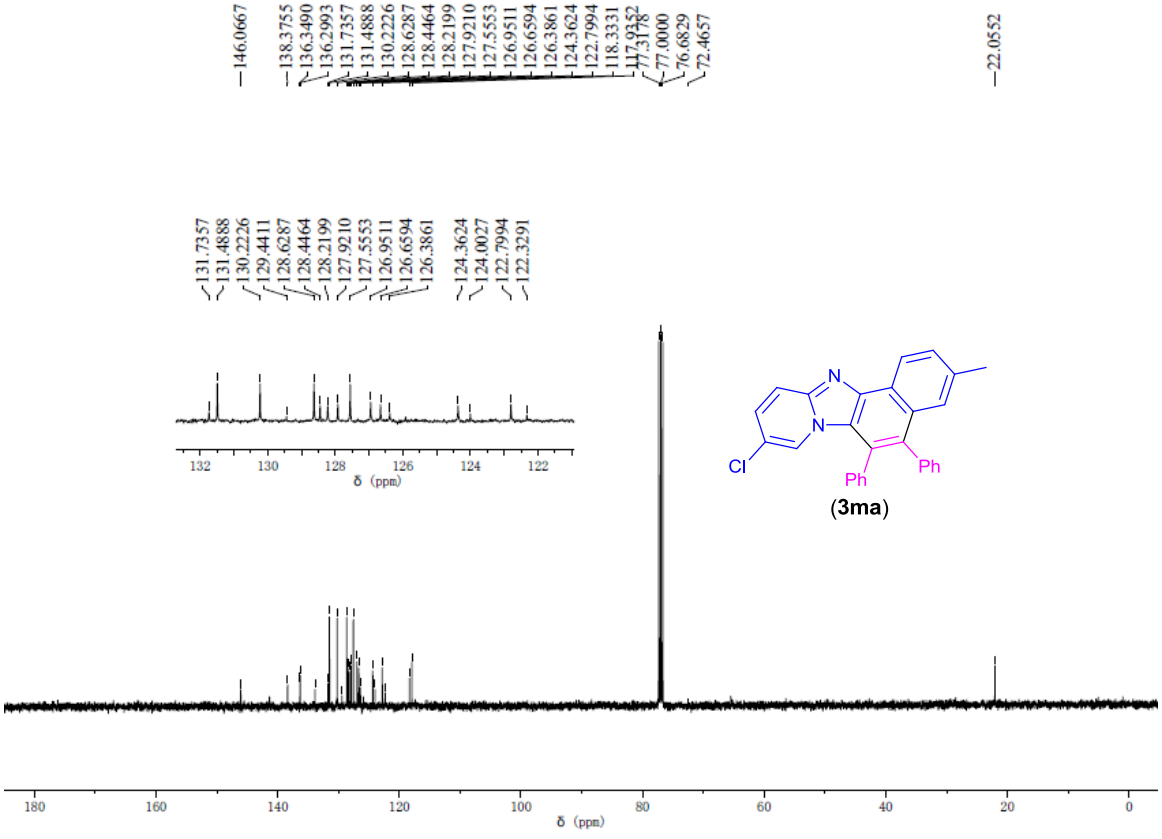

146.0543
138.2333
136.1857
131.4289
130.1819
128.7240
128.6403
128.3273
128.2147
127.9663
127.6683
127.5529
126.7070
126.4384
125.9690
124.3687
122.8609
118.4311
117.9915
77.3174
77.0000
76.6824
134.2075
131.4289
130.1819
128.7240
128.6403
127.9663
127.6683
127.5529
126.7070
126.4384
125.9690
124.3687
123.3119
122.8609
133
131
129
127
125
123
δ (ppm)
N
N
Cl
Ph
Ph
180
160
140
120
100
80
60
40
20
0
δ (ppm)

(**3la**)

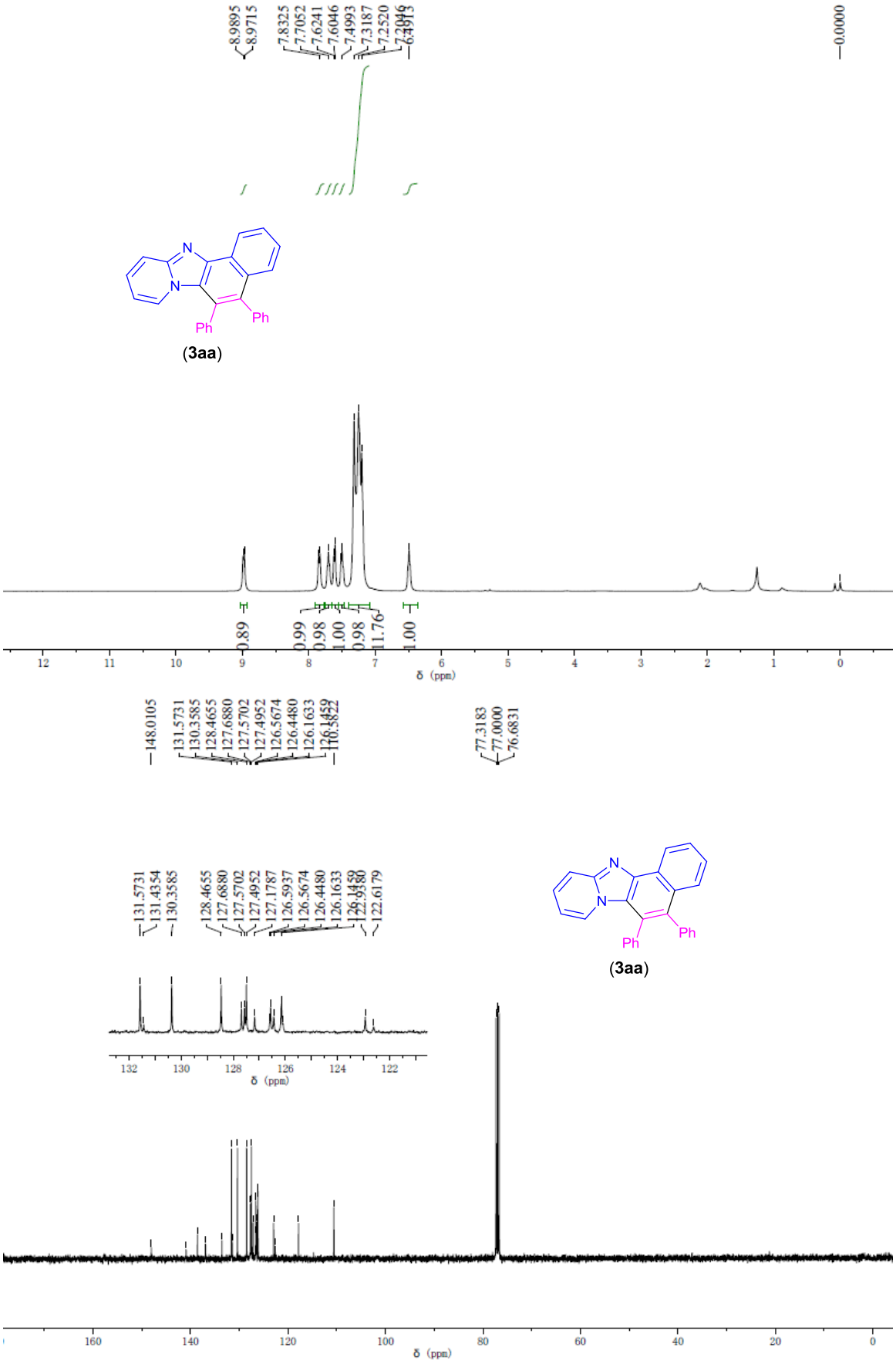

8.8435
8.8229
7.8025
7.7834
7.7594
7.7411
7.5676
7.5470
7.3799
7.3674
7.3557
7.2890
7.2725
7.2565
7.2439
7.2360
7.2062
7.1872
7.1654
2.4504
0.0000
N
N
Cl
Ph
Ph

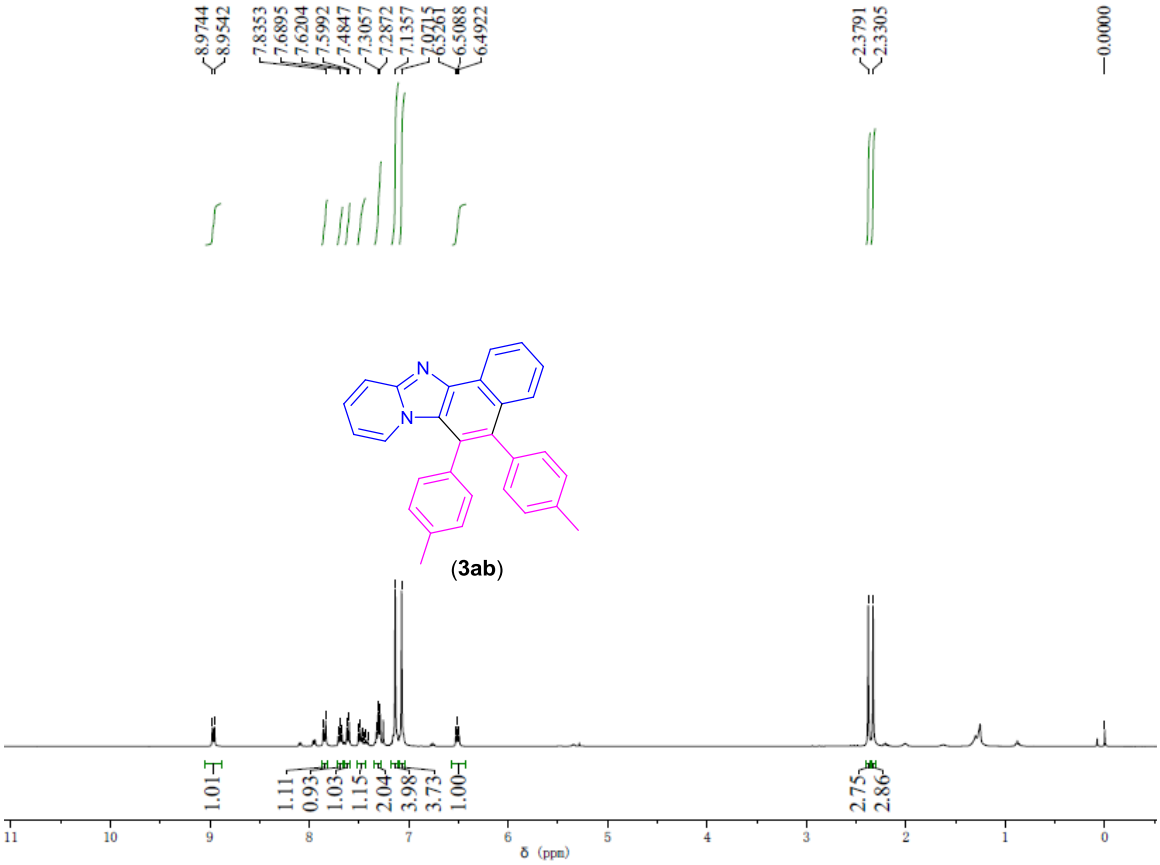
(**3ma**)


1.01
1.36
1.14
2.96
9.77
3.00
δ (ppm)

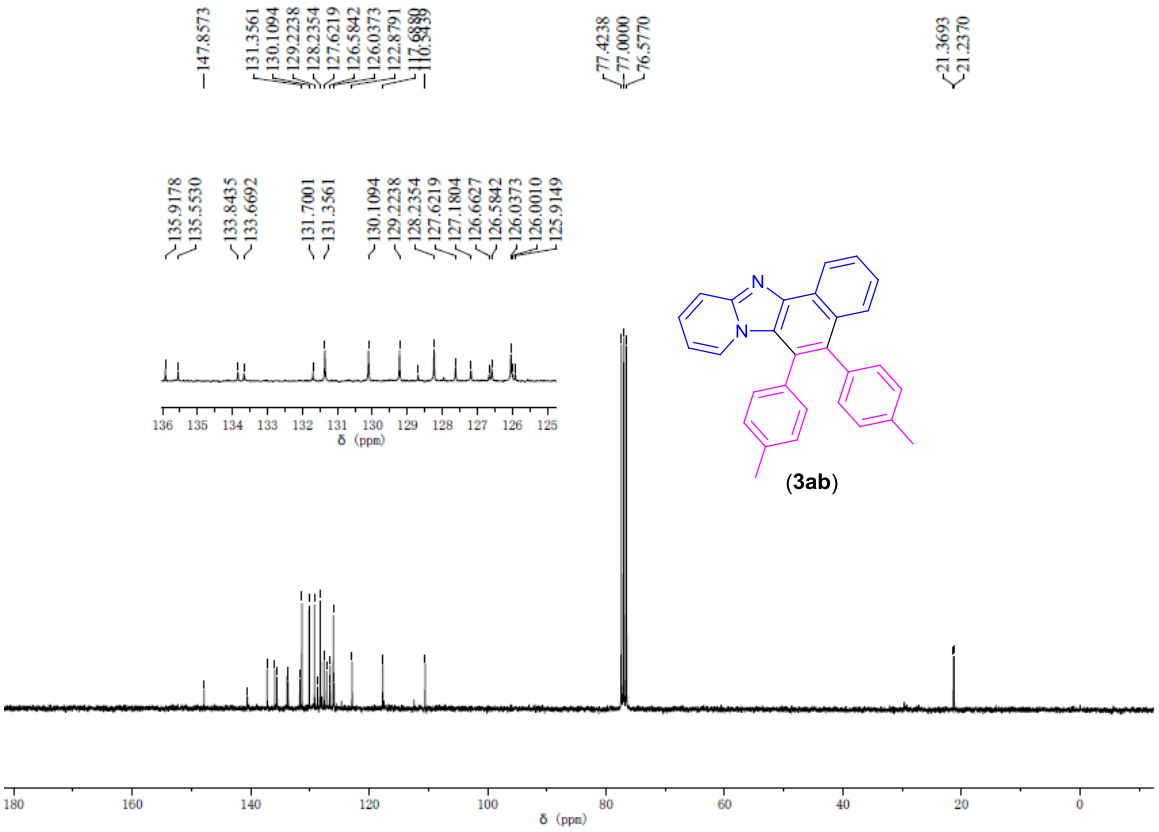

146.0667
138.3755
136.3490
136.2993
131.7357
131.4888
130.2226
128.6287
128.4464
128.2199
127.9210
127.5553
126.9511
126.6594
126.3861
124.3624
122.7994
118.3331
77.0000
76.6829
72.4657
22.0552
131.7357
131.4888
130.2226
129.4411
128.6287
128.4464
128.2199
127.9210
127.5553
126.9511
126.6594
126.3861
124.3624
124.0027
122.7994
122.3291
δ (ppm)
N
N
Cl
Ph
Ph

(**3ma**)

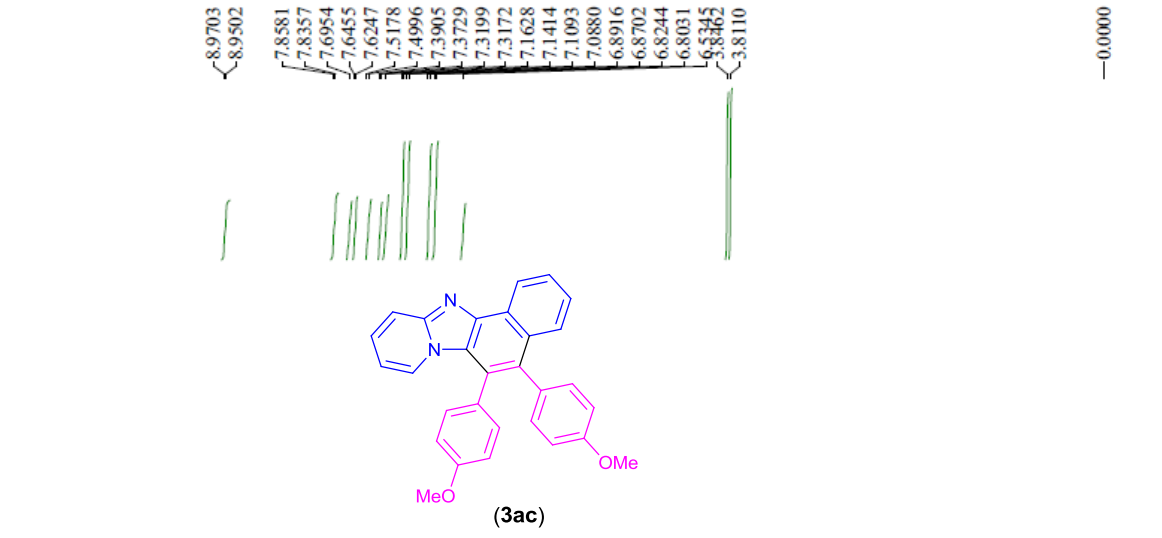

8.9895
8.9715
7.8325
7.7052
7.6241
7.6046
7.4993
7.3187
7.2520
0.0000
N
N
Ph
Ph
(3aa)
0.89
0.99
0.98
1.00
0.98
11.76
1.00
δ (ppm)
148.0105
131.5731
130.3585
128.4655
127.6880
127.5702
127.4952
126.5674
126.4480
126.1633
77.3183
77.0000
76.6831
131.5731
131.4354
130.3585
128.4655
127.6880
127.5702
127.4952
127.1787
126.5937
126.5674
126.4480
126.1633
122.6179
N
N
Ph
Ph
(3aa)
δ (ppm)
δ (ppm)


8.9744
8.9542
7.8353
7.6895
7.6204
7.5992
7.4847
7.3057
7.2872
7.1357
7.0715
6.5261
6.5088
6.4922
2.3791
2.3305
0.0000
1.01
1.11
0.93
1.03
1.15
2.04
3.98
3.73
1.00
2.75
2.86
δ (ppm)

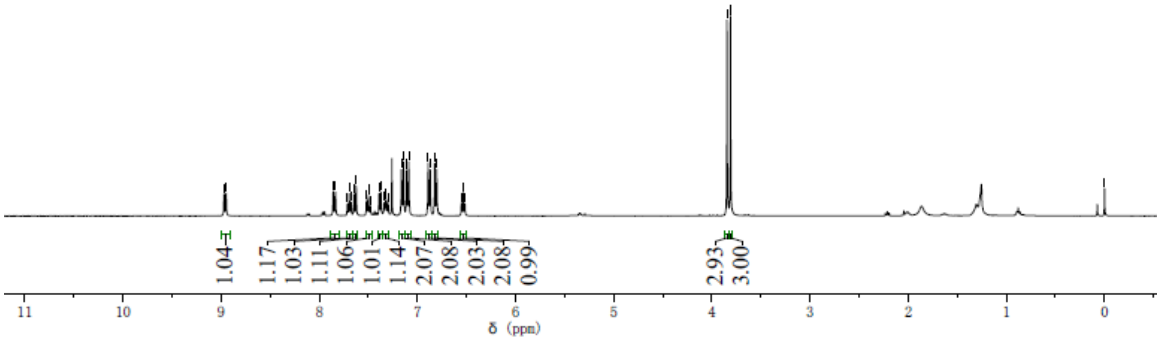
(**3ab**)

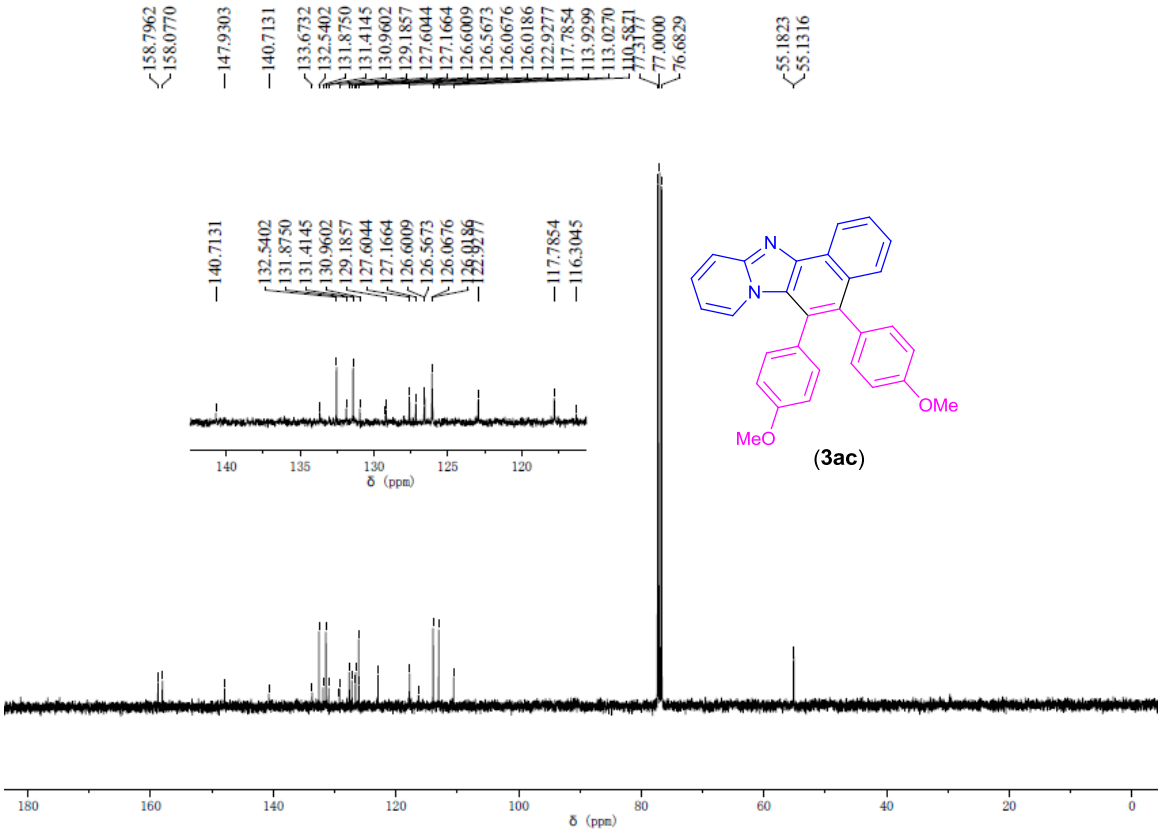

147.8573
131.3561
130.1094
129.2238
128.2354
127.6219
126.5842
126.0373
122.8791
77.4238
77.0000
76.5770
21.3693
21.2370
135.9178
135.5530
133.8435
133.6692
131.7001
131.3561
130.1094
129.2238
128.2354
127.6219
127.1804
126.6627
126.5842
126.0373
126.0010
125.9149
δ (ppm)
δ (ppm)

(**3ab**)

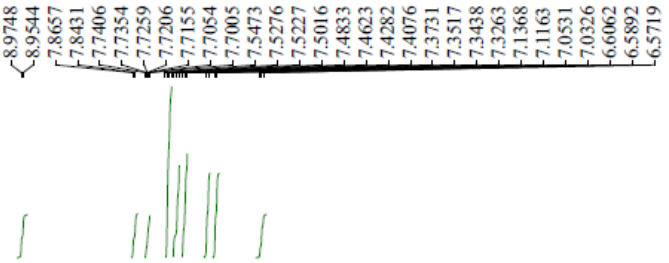

8.9703
8.9502
7.8581
7.8357
7.6954
7.6455
7.6247
7.5178
7.4996
7.3905
7.3729
7.3199
7.3172
7.1628
7.1414
7.1093
7.0880
6.8916
6.8702
6.8244
6.8031
3.8462
3.8110
0.0000
N
N
OMe
MeO

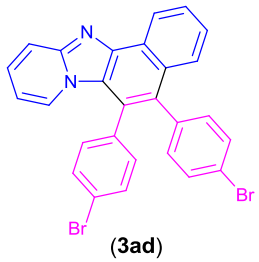
(**3ac**)


1.04
1.17
1.03
1.11
1.06
1.01
1.14
2.07
2.08
2.03
2.08
0.99
2.93
3.00
11
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)

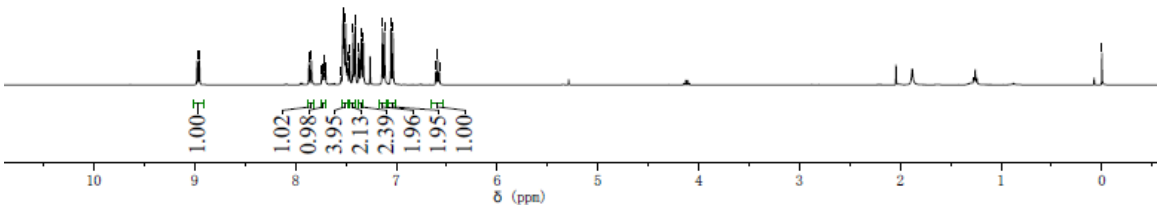

158.7962
158.0770
147.9303
140.7131
133.6732
132.5402
131.8750
131.4145
130.9602
129.1857
127.6044
127.1664
126.6009
126.5673
126.0676
126.0186
122.9277
117.7854
113.9299
113.0270
110.5871
77.3177
77.0000
76.6829
55.1823
55.1316
140.7131
132.5402
131.8750
131.4145
130.9602
129.1857
127.6044
127.1664
126.6009
126.5673
126.0676
117.7854
116.3045
140
135
130
125
120
δ (ppm)
N
N
OMe
MeO
180
160
140
120
100
80
60
40
20
0
δ (ppm)

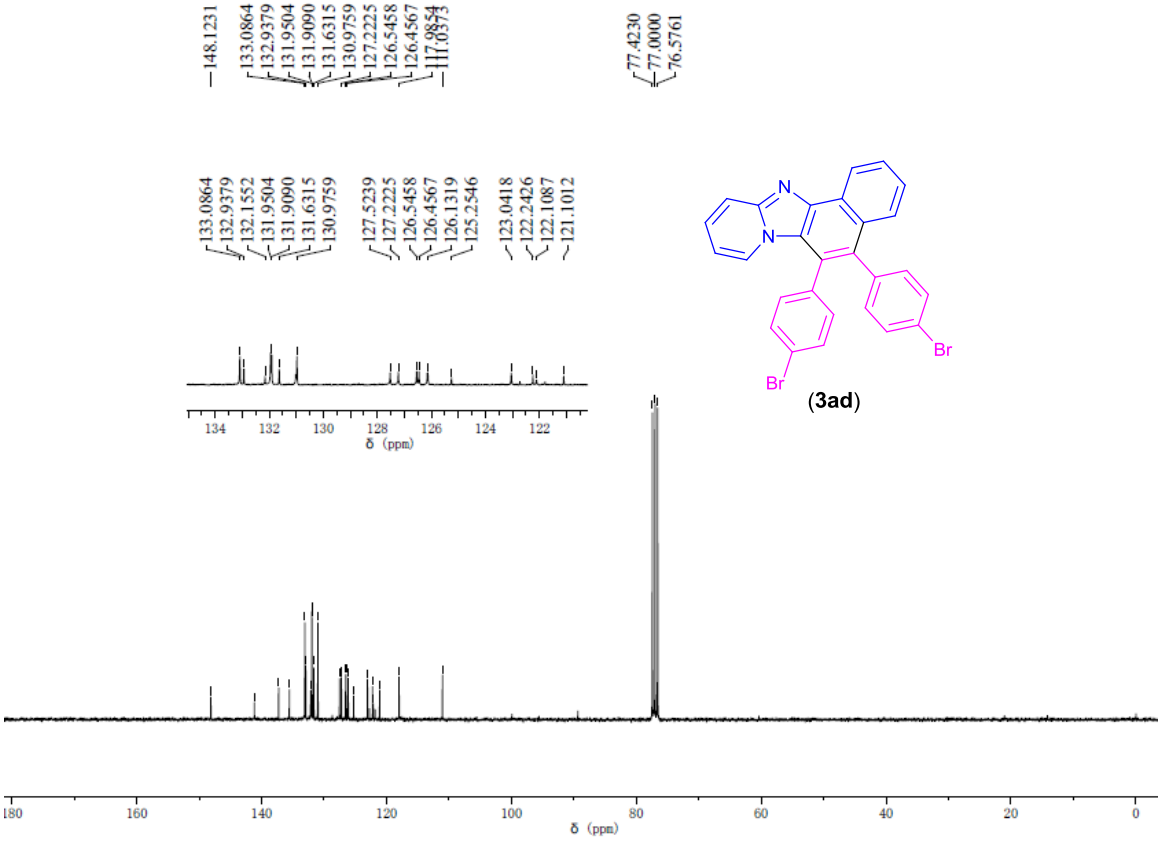
(**3ac**)


8.9748
8.9544
7.8657
7.8431
7.7406
7.7354
7.7259
7.7206
7.7155
7.7054
7.7005
7.5473
7.5276
7.5227
7.5016
7.4833
7.4623
7.4282
7.4076
7.3731
7.3517
7.3438
7.3263
7.1368
7.1163
7.0531
7.0326
6.6062
6.5892
6.5719
0.0000


N
N
Br
Br

(**3ad**)

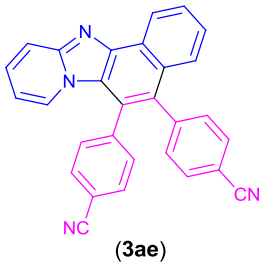

1.00
1.02
0.98
3.95
2.13
2.39
1.96
1.95
1.00
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)


148.1231
133.0864
132.9379
131.9504
131.9090
131.6315
130.9759
127.2225
126.5458
126.4567
117.9854
117.0373
77.4230
77.0000
76.5761
133.0864
132.9379
132.1552
131.9504
131.9090
131.6315
130.9759
127.5239
127.2225
126.5458
126.4567
126.1319
125.2546
123.0418
122.2426
122.1087
121.1012
134
132
130
128
126
124
122
δ (ppm)
180
160
140
120
100
80
60
40
20
0
δ (ppm)

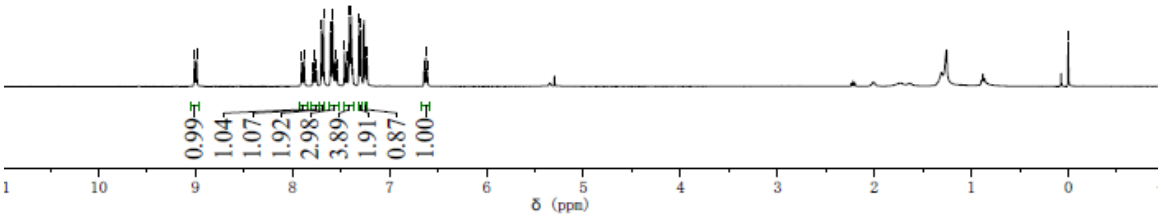
N
N
Br
Br

(**3ad**)

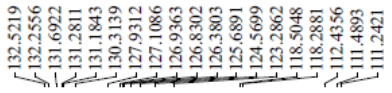

9.0100
8.9897
7.7025
7.6822
7.5878
7.4143
7.3941
7.3137
7.2936
6.6434
6.6265
6.6092
-0.0000

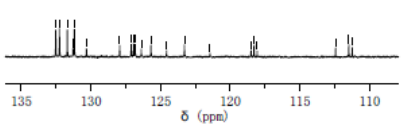

N
N
CN
NC

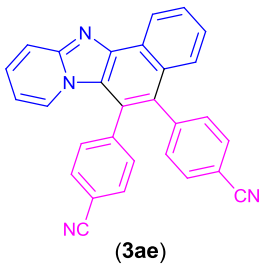
(**3ae**)


0.99
1.04
1.07
1.92
2.98
3.89
1.91
0.87
1.00
δ (ppm)

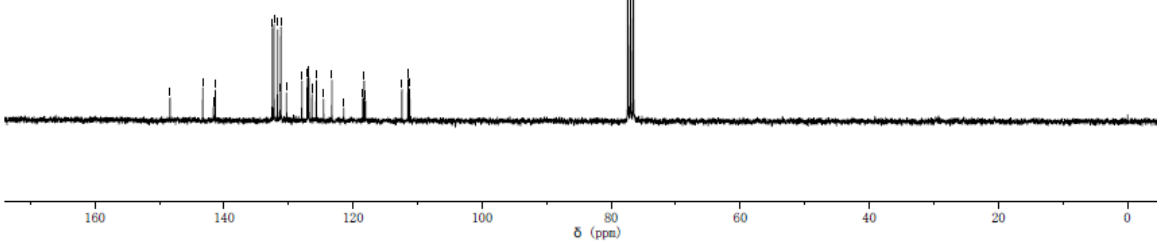

148.3704
143.3003
141.6506
141.3663
132.5219
132.2556
131.6922
131.2811
131.1843
130.3139
127.9312
127.1086
126.9363
126.8302
126.3803
125.6891
123.2862
118.5048
118.2881
112.4356
111.4893
111.2421
77.4231
77.0000
76.5760

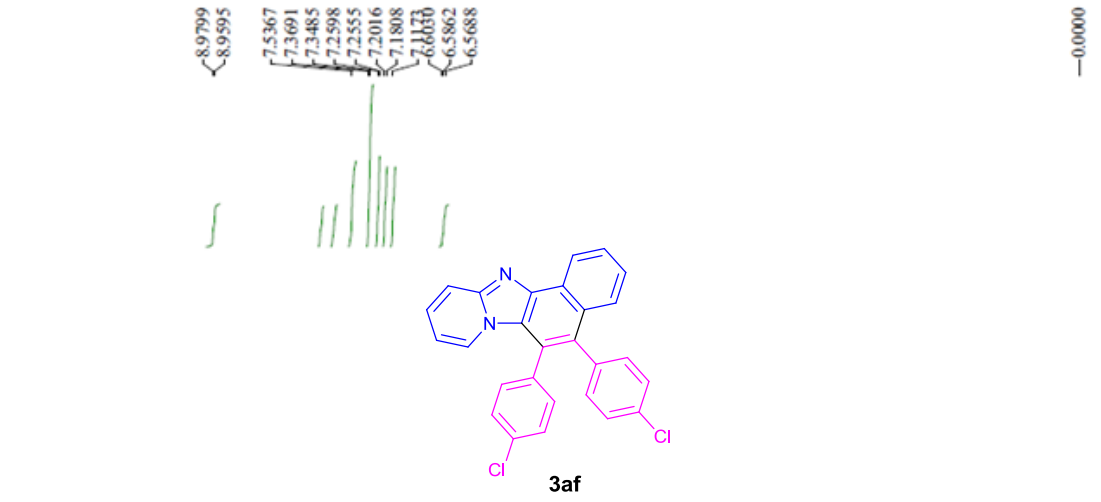

132.5219
132.2556
131.6922
131.2811
131.1843
130.3139
127.9312
127.1086
126.9363
126.8302
126.3803
125.6891
124.5699
123.2862
118.5048
118.2881
112.4356
111.4893
111.2421


135
130
125
120
115
110
δ (ppm)

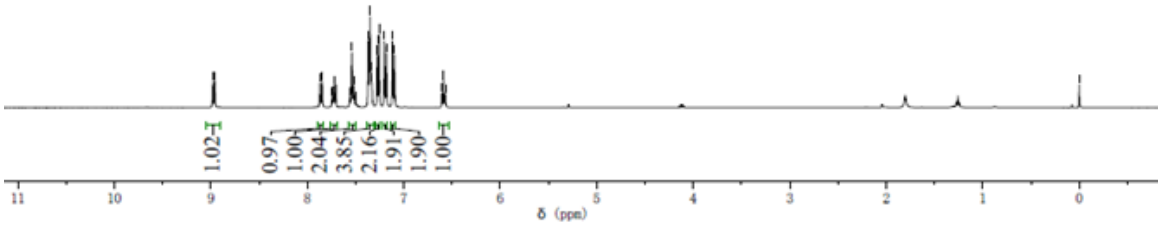

N
N
CN
NC

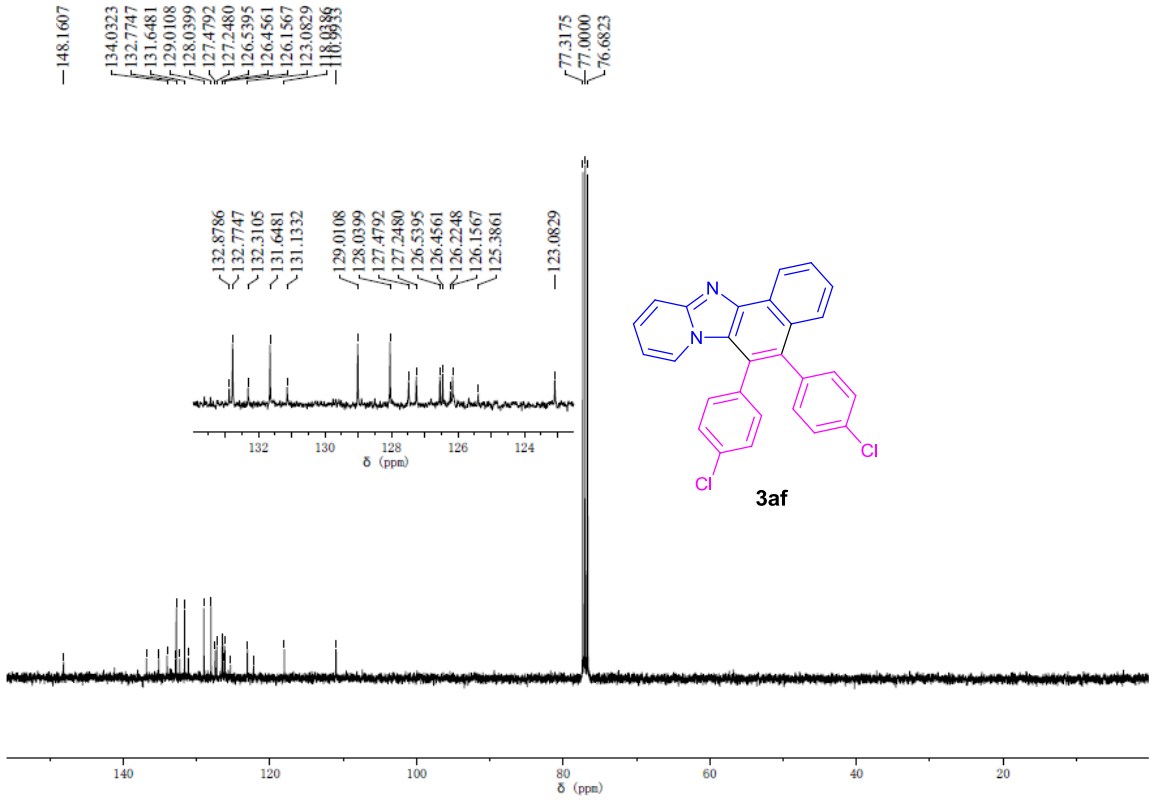
(**3ae**)


160
140
120
100
80
60
40
20
0
δ (ppm)

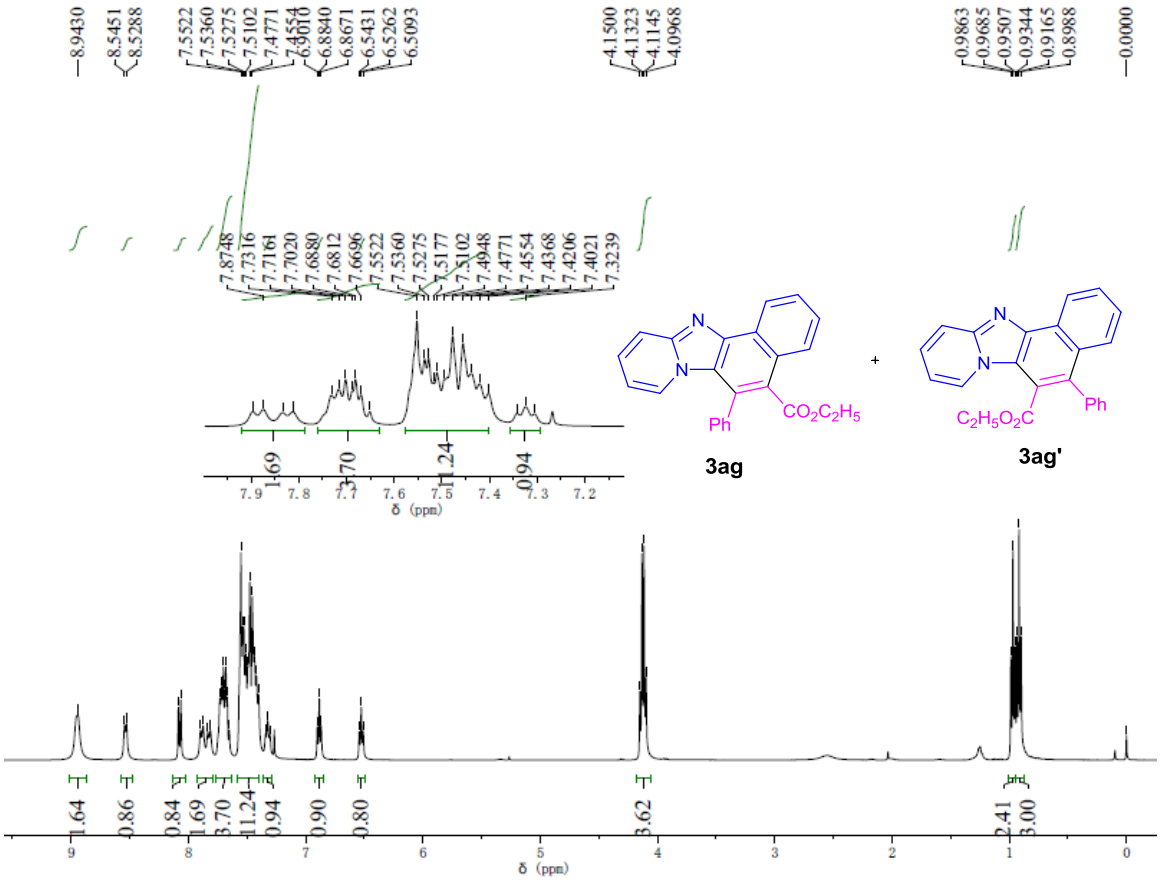

8.9799
8.9595
7.5367
7.3691
7.3485
7.2598
7.2555
7.2016
7.1808
7.1173
6.6030
6.5862
6.5688
0.0000
N
N
Cl
Cl

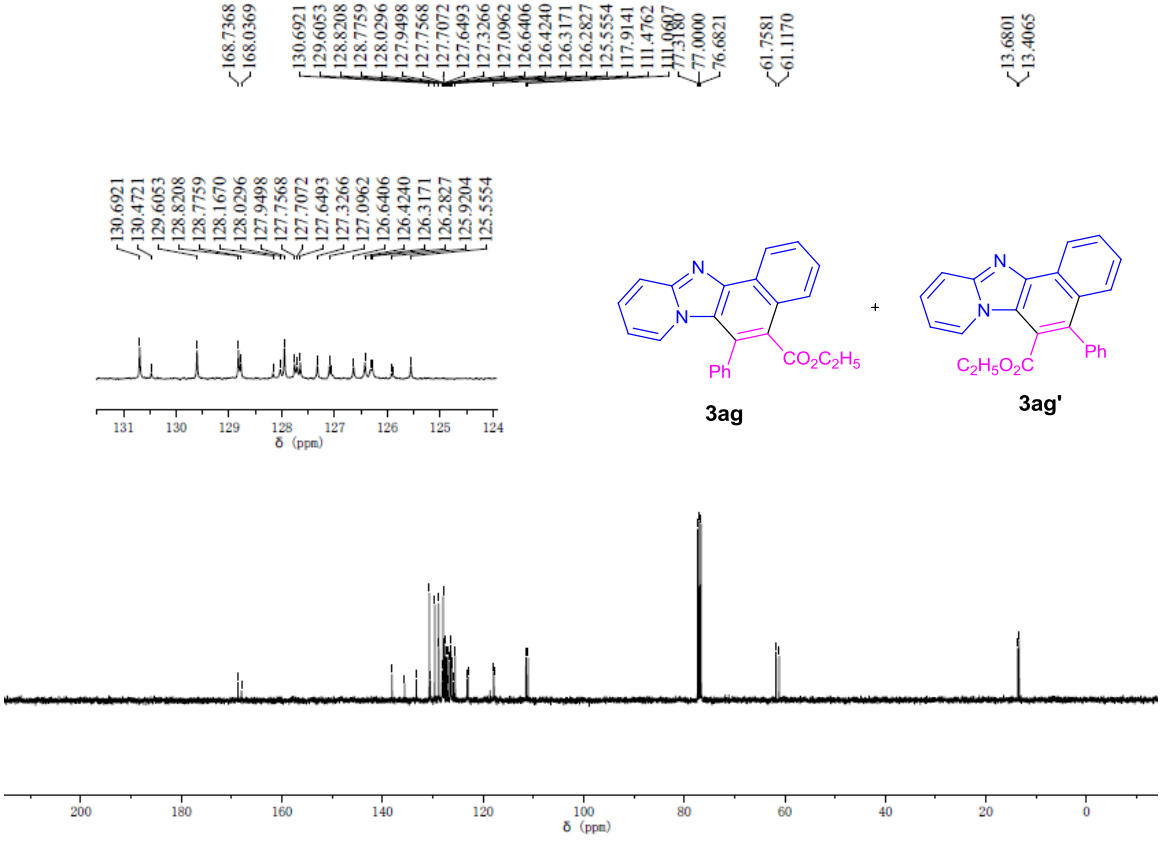
3af

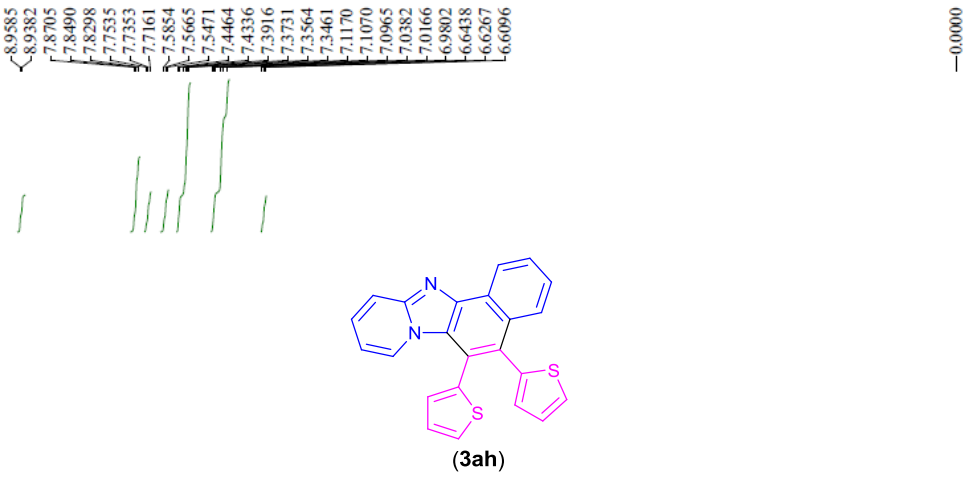

1.02
0.97
1.00
2.04
3.85
2.16
1.91
1.90
1.00
11
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)


148.1607
134.0323
132.7747
131.6481
129.0108
128.0399
127.4792
127.2480
126.5395
126.4561
126.1567
123.0829
77.3175
77.0000
76.6823
132.8786
132.7747
132.3105
131.6481
131.1332
129.0108
128.0399
127.4792
127.2480
126.5395
126.4561
126.2248
126.1567
125.3861
123.0829
132
130
128
126
124
δ (ppm)
N
N
Cl
Cl
140
120
100
80
60
40
20
δ (ppm)

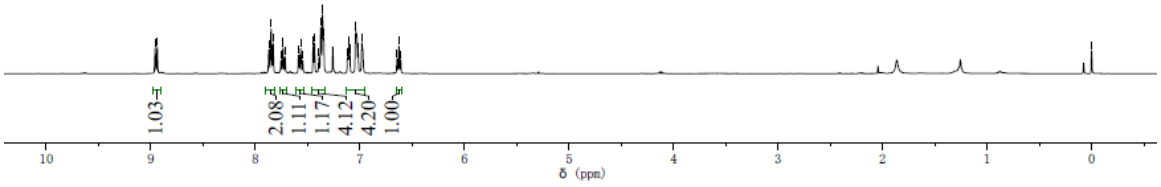
3af

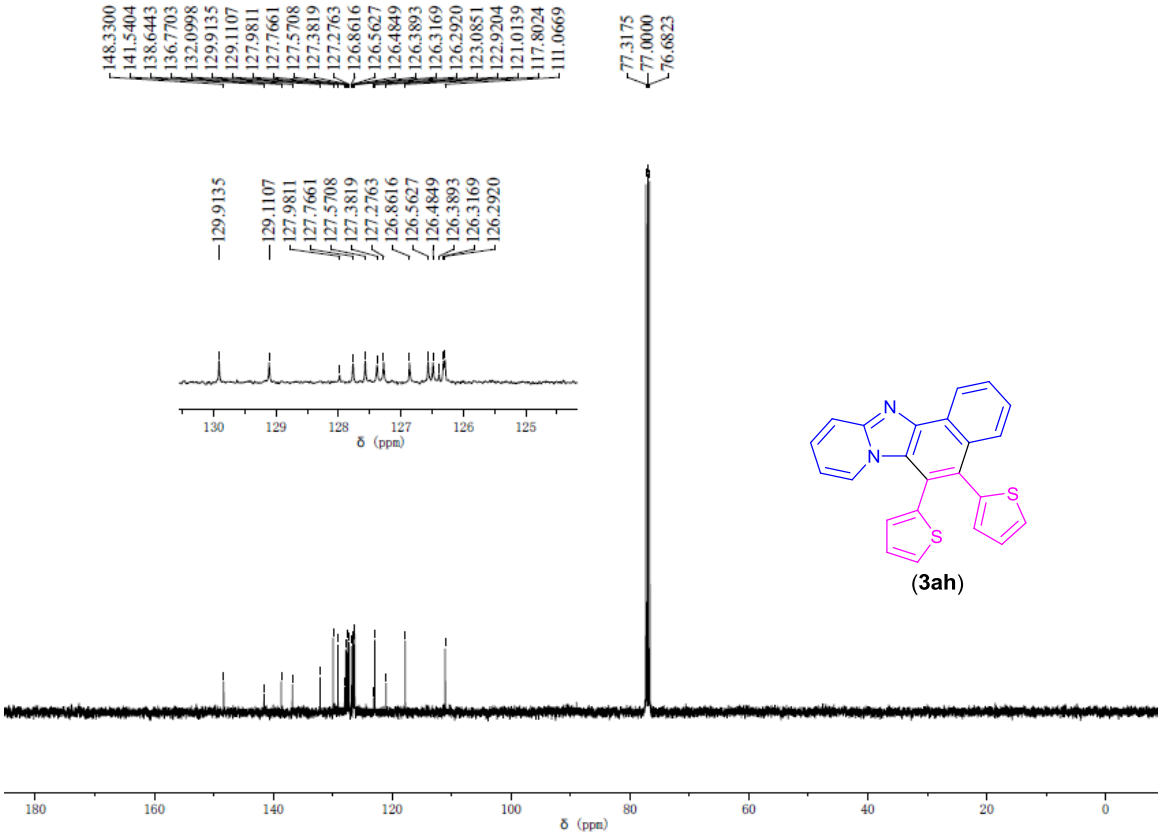

3ag
3ag'
δ (ppm)


3ag
3ag'
δ (ppm)


8.9585
8.9382
7.8705
7.8490
7.8298
7.7535
7.7353
7.7161
7.5854
7.5665
7.5471
7.4464
7.4336
7.3916
7.3731
7.3564
7.3461
7.1170
7.1070
7.0965
7.0382
7.0166
6.9802
6.6438
6.6267
6.6096
0.0000
N
N
S
S

(**3ah**)


1.03
2.08
1.11
1.17
4.12
4.20
1.00
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)


148.3300
141.5404
138.6443
136.7703
132.0998
129.9135
129.1107
127.9811
127.7661
127.5708
127.3819
127.2763
126.8616
126.5627
126.4849
126.3893
126.3169
126.2920
123.0851
122.9204
121.0139
117.8024
111.0669
77.3175
77.0000
76.6823
129.9135
129.1107
127.9811
127.7661
127.5708
127.3819
127.2763
126.8616
126.5627
126.4849
126.3893
126.3169
126.2920
130
129
128
127
126
125
δ (ppm)
N
N
S
S
180
160
140
120
100
80
60
40
20
0
δ (ppm)

(**3ah**)