–Electronic Supporting Information –

Nickel-catalyzed [2+2+2] benzannulation of alkynes: a new route to synthesis of highly substituted naphthalenes

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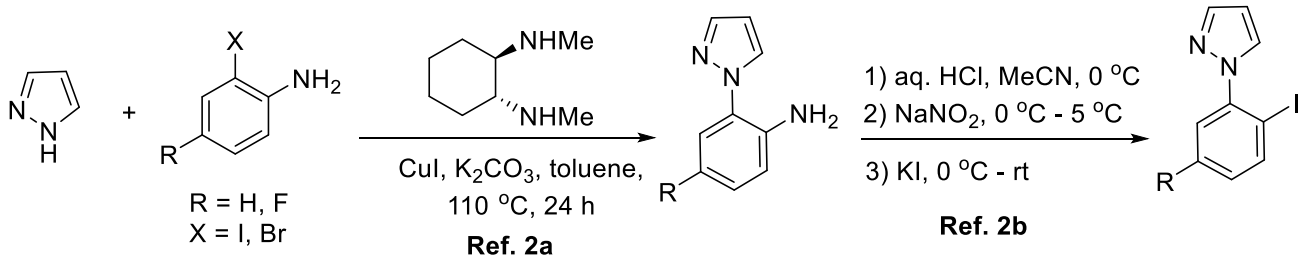
Table of Contents	**Page No**

General information

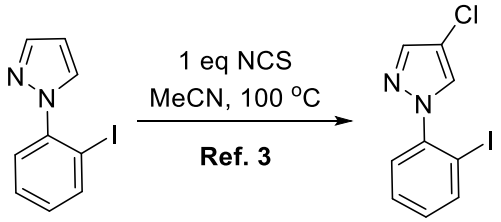
All product mixtures were analyzed by thin layer chromatography using aluminum foil backed silica TLC plates with a fluorescent indicator from Merck. UV-active compounds were detected with a UV lamp (λ = 254 nm). For flash column chromatography, silica gel was used as stationary phase. ^{1}H and ^{13}C NMR spectra were recorded on Bruker (300 MHz and 500 MHz) in deuterated chloroform at 25 °C. Chemical shifts (δ) are reported in ppm, and spin-spin coupling constants (*J*) are given in Hz, while multiplicities are abbreviated by br s (broad singlet), s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). High resolution mass spectra (HRMS) were recorded on Waters Xevo G2S QTof (ESI) instrument.

All solvents were dried according to known methods and distilled prior to use.[1] 1-(2-iodophenyl)-1*H*-pyrazole **1a-b**,[2a-b] 4-chloro-1-(2-iodophenyl)-1*H*-pyrazole **1c,**[3] 1-(2-bromophenyl)-4-phenyl-1*H*-pyrazole **1d,**[4] 2-(2-bromophenyl)imidazo[1,2-*a*]pyridine **4a,**[5] 1-(2-bromophenyl)-4-phenyl-1*H*-1,2,3-triazole **8a**[6] and alkynes **2b-2f**[7] were synthesized according to literature procedures. The nickel(II)complex $NiBr_2$(dppe) was prepared according to the literature protocols.[8] All other reagents were purchased from Sigma-Aldrich, Acros or Alfa Aesar and used without further purification.

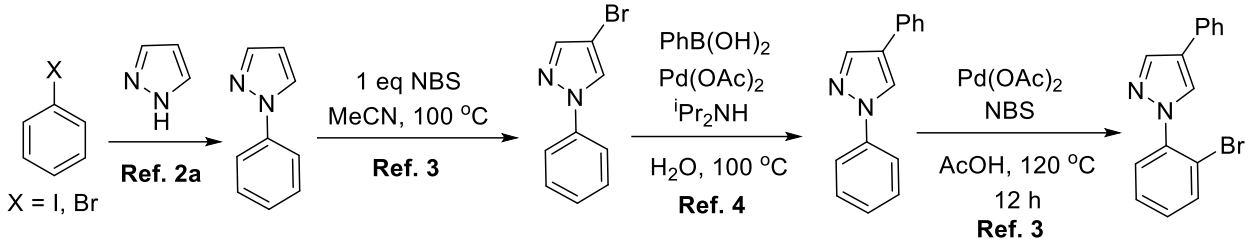
Scheme: S1 Synthesis of 1-(2-iodophenyl)-1*H*-pyrazole (1a-b) [2a-b]



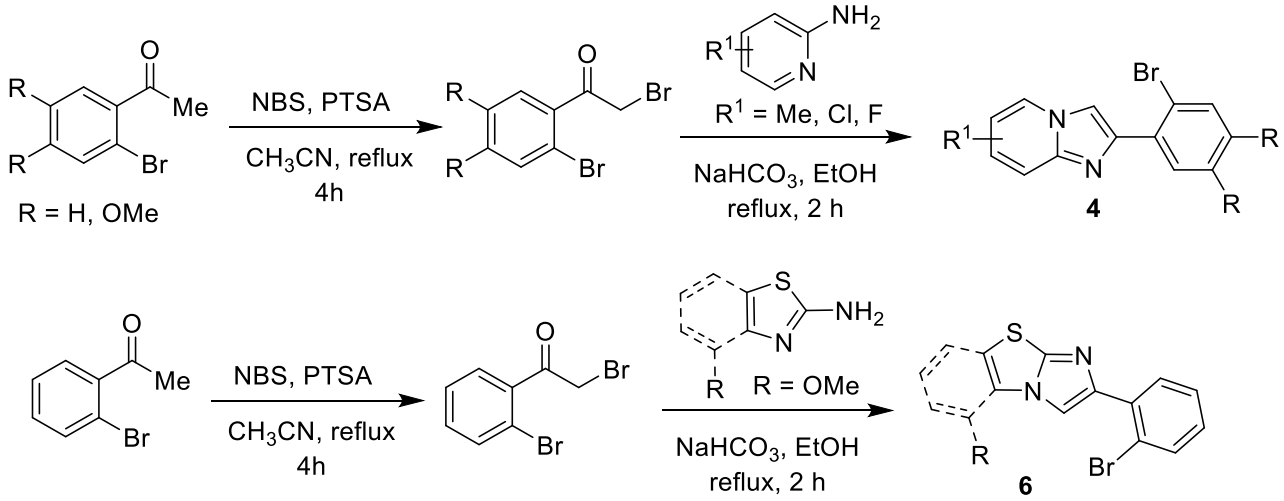
Scheme: S2 Synthesis of 4-chloro-1-(2-iodophenyl)-1*H*-pyrazole (1c) [3]



Scheme: S3 Synthesis of 1-(2-bromophenyl)-4-phenyl-1*H*-pyrazole (1d) [2a, 3, 4]



Scheme: S4 Preparation of 2-(2-bromophenyl)imidazo[1,2-*a*]pyridine (4a-f, 6a-c)[5]

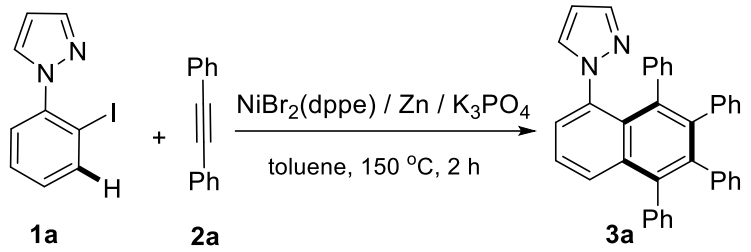


A solution of 2'-bromoacetophenone (2g, 10 mmol), N-bromosuccinimide (1.78g, 10 mmol) and *p*-toluenesulphonic acid (2.59g, 15.0 mmol) in acetonitrile (15 mL) was stirred for 4 h at 85 ^{o}C. Up on completion, the reaction was allowed to cool to room temperature and the solvent was evaporated. The residue was diluted with water and the product was extracted into ethyl acetate (3x15 mL). The organic layer was dried over anhydrous sodium sulphate and the solution was evaporated to dryness. The crude 2-bromo-1-(2-bromophenyl)ethanone (light brown liquid) was subjected to next step without further purifications.

To a solution of 2-bromo-1-(2-bromophenyl)ethanone (2.4g, 9.10 mmol) and sodium bicarbonate (1.14g, 13.65 mmol) in ethanol (20 mL) was added 2-aminopyridine (1g, 9.10 mmol) and the reaction mixture was stirred at 80 ^{o}C for 2 h. After completion (based on TLC), the reaction mass was allowed to cool to room temperature and the solvent were evaporated. The residue was diluted with water and extracted into ethyl acetate (3x15 mL). The organic layer was dried over anhydrous sodium sulphate and the solution was evaporated to dryness. The crude

residue was purified by column chromatography to get pure product **4a**. Similar experimental procedure was applied for the synthesis of **4b-f**, **6a-c**.

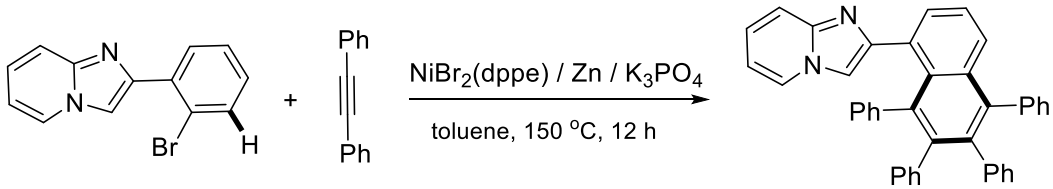
Scheme: S5 General procedure for the nickel-catalyzed benzannulation of 1-(2-iodophenyl)-1*H*-pyrazole with alkynes:



1a **2a** **3a**

To a Schlenk tube (20 mL) equipped with magnetic stir bar were loaded 1-(2-iodophenyl)-1*H*-pyrazole **1a** (0.277 mmol), diphenylacetylene **2a** (0.831 mmol), $NiBr_2$(dppe) (10 mol %), Zn (3 equiv) K_3PO_4 (1 equiv). Then, dry toluene (3 mL) was added to the system via a syringe and the reaction mixture was allowed to stir at 150 °C (oil bath) for 2 h. When the reaction was completed, the mixture was cooled and diluted with CH_2Cl_2 (10 mL). The mixture was filtered through a Celite pad and the Celite pad was washed with dichloromethane (3 x 15 mL). The combined filtrate was concentrated and the residue was purified by a silica gel column chromatography using hexane–EtOAc as eluent to give pure product **3a**. Similar experimental procedure was applied for the synthesis of **3b-l, 5a-k, 7a-e, 9a.**

Scheme: S6 Gram scale synthesis of **5a**

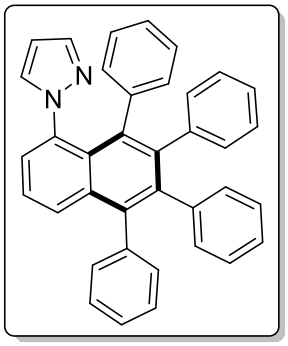


4a: 0.500g (1.83 mmol) **5a:** 0.74 g (74%)

To a Schlenk tube (50 mL) equipped with magnetic stir bar were loaded 2-(2-bromophenyl)imidazo[1,2-*a*]pyridine **4a** (0.5g, 1.830 mmol), diphenylacetylene **2a** (0.978 g, 5.49 mmol), $NiBr_2$(dppe) (10 mol %), Zn (3 equiv) and K_3PO_4 (1 equiv). Then, toluene (10 mL) was added to the system via a syringe and the reaction mixture was allowed to stir at 150 °C for 12 h. When the reaction was completed, the mixture was cooled and diluted with CH_2Cl_2 (20 mL). The mixture was filtered through a Celite pad and the Celite pad was washed with dichloromethane (3 x 20 mL). The combined filtrate was concentrated and the residue was

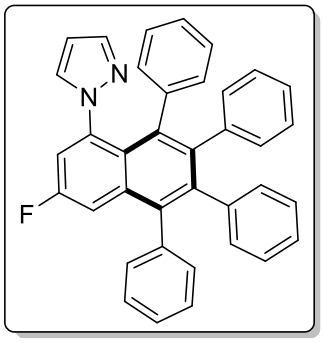
purified by a silica gel column chromatography using hexane–EtOAc as eluent to give pure product **5a** in 74% yield.

1-(5,6,7,8-Tetraphenylnaphthalen-1-yl)-1*H*-pyrazole (3a)



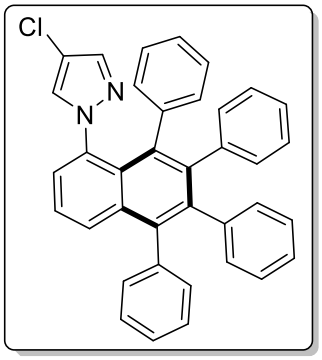
White solid, eluent: (hexane/EtOAc, 95:5), m.p. 170-173 ^{o}C, yield: (112 mg, 85%). **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.79 – 7.76 (m, 1H), 7.44 – 7.41 (m, 2H), 7.27 – 7.16 (m, 8H), 6.83 – 6.77 (m, 12H), 6.66 (s, 2H), 5.74 (d, *J* = 1.8 Hz, 1H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 142.3, 140.3, 140.2, 139.9, 139.8, 139.6, 139.5, 138.7, 138.1, 136.3, 134.3, 132.3, 131.3, 131.2, 131.0, 130.9, 128.9, 127.6 (2C), 126.6, 126.5, 126.2, 126.0, 125.4, 125.1, 125.0, 124.7, 105.9 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{37}H_{26}N_2$ 499.2174, found 499.2171.

1-(3-Fluoro-5,6,7,8-tetraphenylnaphthalen-1-yl)-1*H*-pyrazole (3b)



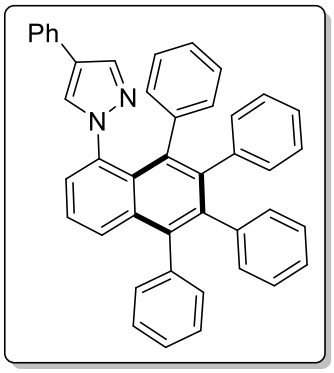
Yellow oil, eluent: (hexane/EtOAc, 95:5), yield: (93 mg, 69%). **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.40 (dd, J_1 = 10.2 Hz, J_2 = 2.4 Hz, 1H), 7.27 - 7.19 (m, 7H), 7.15 (d, *J* = 2.1 Hz, 1H), 6.83 – 6.77 (m, 13H), 6.64 (d, *J* = 2.4 Hz, 2H), 5.75 (d, J = 1.8 Hz, 1H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 158.8 (d, J_{CF} = 245.2 Hz), 141.6 (d, J_{CF} = 2.2 Hz), 140.9, 140.3, 140.1, 139.9 (2C), 139.7, 139.1, 138.3 (d, J_{CF} = 5.2 Hz), 136.5, 135.2 (d, J_{CF} = 9.0 Hz), 132.3, 131.2, 131.1, 130.8, 127.8, 126.9, 126.6, 126.3, 126.1, 125.5, 125.3, 125.1, 124.8, 117.8 (d, J_{CF} = 26.2 Hz), 112.2 (d, J_{CF} = 21.0 Hz), 106.3 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{37}H_{25}FN_2$ 517.2080, found 517.2079.**^{19}F NMR (471 MHz, CDCl$_3$)** δ -114.64 (s) ppm.

4-Chloro-1-(5,6,7,8-tetraphenylnaphthalen-1-yl)-1*H*-pyrazole (3c)



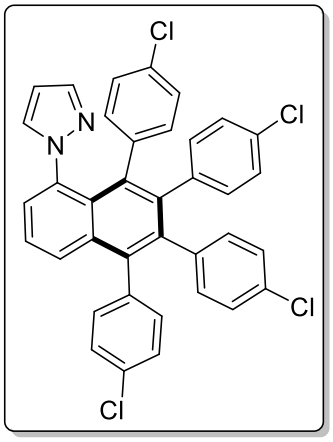
White solid, eluent: (hexane/EtOAc, 95:5), m.p. 185-188 ºC, yield: (92 mg, 70%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.80 (d, *J* = 5.4 Hz, 1H), 7.42 (d, *J* = 4.5 Hz, 2H), 7.26 – 7.23 (m, 6H), 7.09 (s, 1H), 7.03 (s, 1H), 6.83 – 6.78 (m, 13H), 6.66 (s, 1H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 142.5, 140.21, 140.0, 139.5, 139.1, 138.9, 138.2, 137.5, 135.9, 134.3, 131.2, 131.1, 131.0, 130.8, 129.5, 127.7, 127.6, 126.7, 126.5, 126.3, 125.4 (2C), 125.2, 124.7, 110.4 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{37}H_{25}ClN_2$ 533.1785, found 533.1793.

4-Phenyl-1-(5,6,7,8-tetraphenylnaphthalen-1-yl)-1*H*-pyrazole (3d)



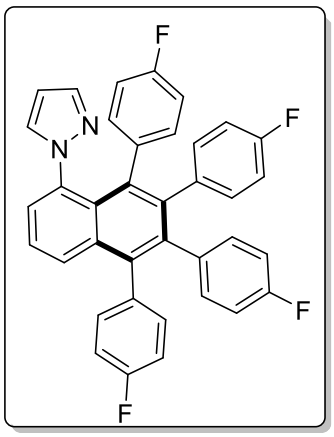
White solid, eluent: (hexane/EtOAc, 95:5), m.p. 188-190 ºC, yield: (85 mg, 59%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.50 – 7.41 (m, 4H), 7.31 – 7.19 (m, 10H), 7.06 (d, *J* = 7.8 Hz, 1H), 6.85 – 6.81 (m, 7H), 6.77 – 6.72 (m, 7H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 142.4, 142.3, 140.3, 140.2 (2C), 140.0, 139.9, 139.6, 139.5, 139.3, 138.9, 137.9, 137.7, 137.5, 137.4, 136.2, 134.4, 132.7, 131.7, 131.3, 131.2, 131.0, 129.8, 129.3, 129.1, 128.5, 127.6, 127.2, 126.6, 126.5, 126.3, 126.0, 125.7, 125.4, 125.2, 125.1, 124.8, 123.2, 122.1, 119.7 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{43}H_{30}N_2$ 575.2487, found 575.2488.

1-(5,6,7,8-Tetrakis(4-chlorophenyl)naphthalen-1-yl)-1*H*-pyrazole (3e)



Yellow solid, eluent: (hexane/EtOAc, 95:5), m.p. 282-284 ^{o}C, yield: (129 mg, 73%). **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.71 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.29 – 7.27 (m, 3H), 7.16 – 7.11 (m, 3H), 6.92 – 6.67 (m, 10H), 6.56 (s, 2H), 5.88 (d, *J* = 1.8 Hz, 1H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 140.7, 140.3, 138.4, 138.1, 138.0, 137.4, 134.3, 133.2, 132.3, 132.2, 132.1, 131.9, 131.6, 128.7, 128.2, 127.9, 127.3, 127.0, 126.5, 125.5, 106.3 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{37}H_{22}Cl_4N_2$ 635.0615, found 635.0614.

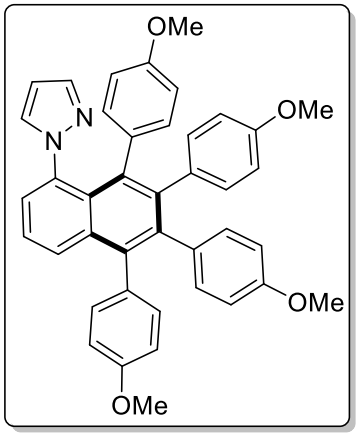
1-(5,6,7,8-Tetrakis(4-fluorophenyl)naphthalen-1-yl)-1*H*-pyrazole (3f)



White solid, eluent: (hexane/EtOAc, 95:5), m.p. 222-227 ^{o}C, yield: (109 mg, 69%). **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.74 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.27 (s, 1H), 7.18 – 7.14 (m, 3H), 7.02 – 6.96 (m, 2H), 6.79 – 6.69 (m, 4H), 6.64 – 6.47 (m, 8H), 5.87 (d, *J* = 1.8 Hz, 1H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 161.8 (d, J_{CF} = 245.2 Hz), 160.9 (d, J_{CF} = 244.5 Hz), 160.8 (d, J_{CF} = 243.0 Hz), 160.7 (d, J_{CF} = 243.7 Hz), 141.5, 140.2, 139.1, 138.2 (d, J_{CF} =

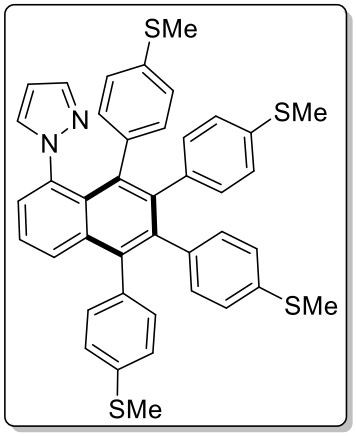
22.5 Hz), 136.8, 136.0, 135.9 (2C), 135.8 (d, J_{CF} = 3.7 Hz), 135.2, 135.1 (d, J_{CF} = 3.7 Hz), 134.4, 132.7, 132.6, 132.5, 132.3, 132.2, 132.1, 128.8, 128.0, 127.9, 125.3, 114.9 (d, J_{CF} = 21.7 Hz), 114.1, 113.8, 113.5, 113.2 (d, J_{CF} = 21.0 Hz), 106.2 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{37}H_{22}F_4N_2$ 571.1797, found 571.1801.**^{19}F NMR (471 MHz, $CDCl_3$)** δ -114.99 (s), -116.17 (s), -116.53 (s), -117.25 (s) ppm.

1-(5,6,7,8-Tetrakis(4-methoxyphenyl)naphthalen-1-yl)-1*H*-pyrazole (3g)



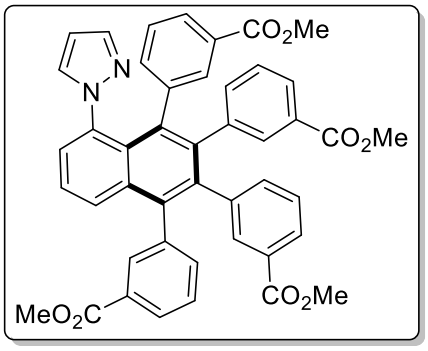
Brown solid, eluent: (hexane/EtOAc, 80:20), m.p. 106-108 ºC, yield: (94 mg, 55%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.67 (dd, *J* = 10.5, 6.5 Hz, 1H), 7.31 (d, *J* = 3.7 Hz, 2H), 7.18 (d, *J* = 5.7 Hz, 2H), 7.04 (t, *J* = 8.0 Hz, 3H), 6.72 (d, *J* = 8.4 Hz, 2H), 6.61 (d, *J* = 8.2 Hz, 3H), 6.55 (s, 1H), 6.43 (d, *J* = 8.4 Hz, 2H), 6.33 (d, *J* = 8.3 Hz, 2H), 6.26 (t, *J* = 8.9 Hz, 3H), 5.70 (s, 1H), 3.72 (s, 3H), 3.58 (s, 3H), 3.54 (s, 3H), 3.52 (s, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 158.4, 158.2, 157.1, 156.9, 142.5, 140.1, 140.0, 139.8, 138.5, 137.9, 135.9, 134.7, 133.2, 133.0, 132.8, 132.6, 132.3, 132.2, 132.1, 132.0, 131.8, 128.8, 127.3, 124.4, 113.6, 113.4, 113.2, 112.7, 112.4, 112.2, 112.0, 105.8, 55.1 (2C), 54.9 (2C) ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{41}H_{34}N_2O_4$ 619.2597, found 619.2562.

1-(5,6,7,8-Tetrakis(4-(methylthio)phenyl)naphthalen-1-yl)-1*H*-pyrazole (3h)



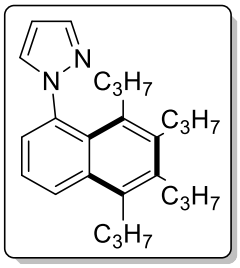
Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 184-186 ^{o}C, yield: (112 mg, 59%). **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.75 (dd, J_1 = 6.3 Hz, J_2 = 3.3Hz, 1H), 7.43 – 7.41 (m, 2H), 7.27 – 7.7.25 (m, 2H), 7.19 – 7.10 (m, 5H), 6.81 – 6.67 (m, 10H), 6.54 – 6.52 (m, 1H), 5.81 (s, 1H), 2.49 (s, 3H), 2.35 (s, 3H), 2.32 (s, 3H), 2.29 (s, 3H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 141.6, 140.0, 139.2, 138.4, 137.9, 137.1, 136.8, 136.2, 135.9, 135.5, 135.2, 134.8, 134.5, 132.2, 131.6, 131.5, 131.3, 128.8, 127.7, 126.0, 125.7, 125.4 (2C), 124.9, 106.0, 16.6, 16.1, 15.9, 15.7 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{41}H_{34}N_2S_4$ 683.1683, found 683.1686.

Tetramethyl 3,3',3'',3'''-(5-(1*H*-pyrazol-1-yl)naphthalene-1,2,3,4-tetrayl)tetrabenzoate (3i)



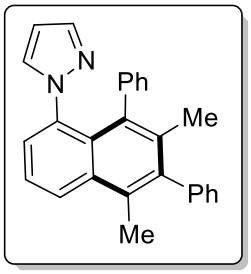
Yellow oil, eluent: (hexane/EtOAc, 70:30), yield: (116 mg, 57%). **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.90 (d, J = 6.6 Hz, 2H), 7.72 (d, J = 7.5 Hz, 1H), 7.49 – 7.39 (m, 10H), 7.28 – 7.17 (m, 2H), 7.03 – 6.84 (m, 6H), 5.74 (s, 1H), 3.89 (s, 3H), 3.84 (s, 3H), 3.77 (m, 6H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 166.8, 166.7, 166.5, 166.4, 141.2, 140.2, 139.7 (2C), 139.2, 139.0 (2C), 138.8, 138.4, 138.0, 135.2, 135.0, 134.1, 132.3, 132.2, 132.1 (2C), 132.0, 131.9, 130.0, 129.9, 128.9, 128.8, 128.6, 128.3, 128.0, 127.8, 127.2, 126.9, 126.8, 126.4, 126.3, 125.6, 106.4, 51.9 (2C), 51.7, 51.6 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{45}H_{34}N_2O_8$ 731.2393, found 731.2388.

1-(5,6,7,8-Tetrapropylnaphthalen-1-yl)-1*H*-pyrazole (3j)



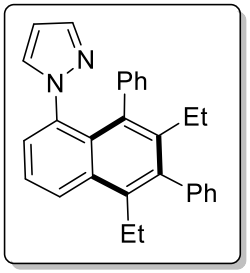
Brown oil, eluent: (hexane/EtOAc, 97:3), yield: (66 mg, 66%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 8.03 (d, *J* = 8.7 Hz, 1H), 7.66 – 7.65 (m, 1H), 7.54 – 7.53 (m, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.17 – 7.15 (m, 1H), 6.38 (t, *J* = 2.1 Hz, 1H), 2.99 2.94 (m, 2H), 2.69 – 2.58 (m, 4H), 1.66 – 1.46 (m, 10H), 1.07 – 0.94 (m, 9H), 0.55 (t, *J* = 7.2 Hz, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 140.1, 139.9, 138.0, 137.3, 134.3, 134.2, 133.4, 131.9, 127.8, 126.3, 126.2, 123.1, 106.2, 32.9, 32.5, 31.8, 30.8, 26.5, 24.9, 24.7, 24.5, 14.9, 14.8, 14.7, 14.2 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{25}H_{34}N_2$ 363.2800, found 363.2777.

1-(5,7-dimethyl-6,8-diphenylnaphthalen-1-yl)-1*H*-pyrazole (3k)



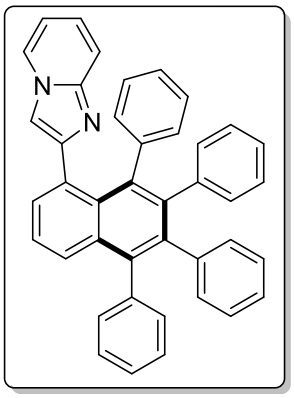
White solid, eluent: (hexane/EtOAc, 97:3), m.p. 113-116 ^{o}C, yield: (66 mg, 63%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.34 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.60 (dd, *J* = 8.4, 7.3 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.40 (dd, *J* = 7.1, 1.1 Hz, 1H), 7.34 (s, 2H), 7.29 (s, 2H), 7.18 – 7.14 (m, 2H), 7.09 (dd, *J* = 10.4, 4.3 Hz, 1H), 7.04 (s, 2H), 5.85 (t, *J* = 2.0 Hz, 1H), 2.55 (s, 3H), 1.70 (s, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 142.2, 141.1, 140.7, 139.6, 137.8, 135.8, 134.8, 133.2, 132.5, 131.2, 128.5, 128.4, 128.1, 127.7, 127.1, 126.8, 126.2, 125.5, 124.1, 105.8, 20.2, 17.5 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{27}H_{22}N_2$ 375.1861, found 375.1835.

1-(5,7-diethyl-6,8-diphenylnaphthalen-1-yl)-1*H*-pyrazole (3l)



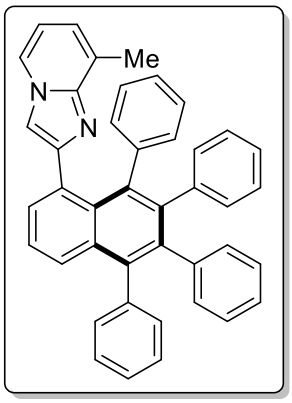
White solid, eluent: (hexane/EtOAc, 97:3), m.p. 147-150 ºC, yield: (67 mg, 60%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 8.28 (d, *J* = 8.7 Hz, 1H), 7.53 – 7.37 (m, 4H), 7.28 – 7.52 (m, 5H), 7.07 – 7.05 (m, 5H), 5.79 (d, *J* = 1.8 Hz, 1H), 2.88 (q, *J* = 7.5 Hz, 2H), 2.10 (s, 2H), 1.20 (t, *J* = 7.5 Hz, 3H), 0.56 (t, *J* = 7.5 Hz, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 141.9, 141.3, 140.2, 140.1, 139.5, 138.2, 138.1, 134.6, 132.4, 132.1, 129.7, 129.1, 127.9, 127.8, 127.5, 127.1, 126.8, 126.3, 125.5, 124.1, 105.8, 24.7, 23.8, 15.4, 14.9 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{29}H_{26}N_2$ 403.2174, found 403.2186.

2-(5,6,7,8-Tetraphenylnaphthalen-1-yl)imidazo[1,2-*a*]pyridine (5a)



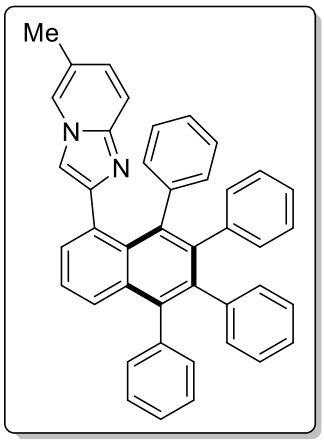
Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 203-206 ºC, yield: (120 mg, 80%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.73 – 7.70 (m, 2H), 7.60 (dd, J_1 = 7.5 H_Z, J_2 = 1.2 H_Z, 1H), 7.46 – 7.41 (m, 1H), 7.36 – 7.34 (m, 1H), 7.27 – 7.16 (m, 5H), 7.0 (t, *J* = 7.8 H_Z, 1H), 6.87 – 6.76 (m, 8H), 6.75 – 6.68 (m, 5H), 6.60 (t, *J* = 6.0 H_Z, 1H), 6.52 (t, *J* = 7.2 H_Z, 2H), 6.44 – 6.39 (m, 1H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 147.2, 143.6, 141.0, 140.8, 140.7, 140.1, 138.9, 138.7, 138.1, 133.7, 133.3, 131.9, 131.4 (2C), 131.2, 131.1, 128.0, 127.4, 126.4, 126.3, 126.1, 125.1, 124.9, 124.8, 124.6 (2C), 124.1, 123.4, 117.2, 112.4, 111.5 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{41}H_{28}N_2$ 549.2331, found 549.2327.

8-Methyl-2-(5,6,7,8-tetraphenylnaphthalen-1-yl)imidazo[1,2-*a*]pyridine (5b)



Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 228-231 ºC, yield: (100 mg, 68%). **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.72 (d, J = 8.4 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.45 – 7.40 (m, 1H), 7.26 – 7.18 (m, 5H), 6.95 (s, 1H), 6.85 – 6.81 (m, 8H), 6.75 – 6.67 (m, 5H), 6.55 – 6.45 (m, 3H), 6.40 – 6.35 (m, 1H), 2.48 (s, 3H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 146.9, 144.2, 140.9, 140.8 (2C), 140.2, 139.0, 138.7, 138.3, 133.8, 133.4, 132.0, 131.4, 131.2 (2C), 128.1, 127.4, 127.1, 126.4, 126.3, 126.1, 125.1, 124.8, 124.6, 124.5, 124.0, 122.5, 122.2, 112.7, 111.5, 17.0 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{42}H_{30}N_2$ 563.2487, found 563.2459.

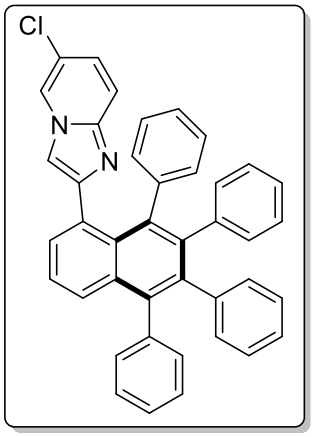
6-Methyl-2-(5,6,7,8-tetraphenylnaphthalen-1-yl)imidazo[1,2-*a*]pyridine (5c)



Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 218-220 ºC, yield: (103 mg, 70%). **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.61 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.50 (dd, *J* = 6.9, 1.2 Hz, 1H), 7.42 (s, 1H), 7.34 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.19 (s, 1H), 7.18 – 7.13 (m, 4H), 7.13 – 7.09 (m, 1H), 6.81 (d, *J* = 9.2 Hz, 1H), 6.80 – 6.64 (m, 11H), 6.63 – 6.57 (m, 2H), 6.44 (t, *J* = 7.6 Hz, 2H), 6.33 (t, *J* = 7.4 Hz, 1H), 2.18 (s, 3H) ppm. **^{13}C NMR (125 MHz, CDCl$_3$)** δ 141.0, 140.7 (2C), 140.0, 138.9, 138.6, 138.0, 133.6, 131.9, 131.4, 131.3, 131.2, 131.1, 128.0, 127.4, 126.8, 126.4, 126.3, 126.1,

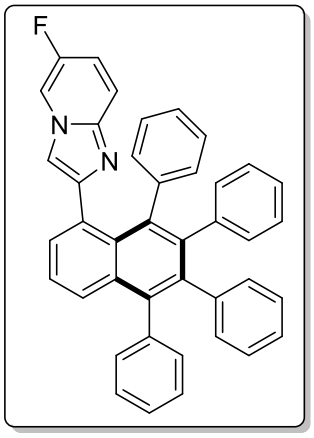
125.1, 125.0, 124.9, 124.6, 124.2, 122.3, 116.4, 112.2, 17.5 ppm. **HRMS (ESI-TOF) m/z:** [M + H]$^+$ Calcd for $C_{42}H_{30}N_2$ 563.2487, found 563.2497.

6-Chloro-2-(5,6,7,8-tetraphenylnaphthalen-1-yl)imidazo[1,2-*a*]pyridine (5d)



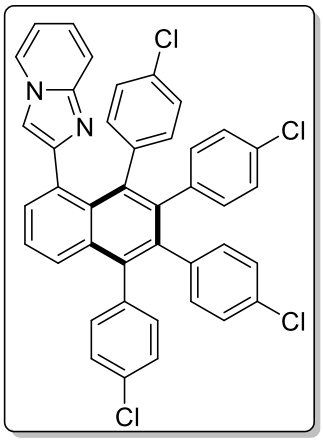
Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 98-100 ^{o}C, yield: (178 mg, 73%). **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.77 (d, *J* = 1.4 Hz, 1H), 7.71 (dd, *J* = 8.5, 1.2 Hz, 1H), 7.55 (dd, *J* = 6.9, 1.2 Hz, 1H), 7.42 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.29 (d, *J* = 9.5 Hz, 1H), 7.26 (s, 1H), 7.23 (dd, *J* = 9.1, 4.0 Hz, 4H), 7.20 – 7.17 (m, 1H), 7.00 (dd, *J* = 9.5, 1.9 Hz, 2H), 6.85 (s, 1H), 6.83 (d, *J* = 3.3 Hz, 1H), 6.82 (d, *J* = 4.6 Hz, 1H), 6.79 (d, *J* = 1.6 Hz, 2H), 6.78 (d, *J* = 1.4 Hz, 2H), 6.76 – 6.74 (m, 1H), 6.74 (d, *J* = 1.8 Hz, 1H), 6.67 (dd, *J* = 7.0, 2.6 Hz, 2H), 6.54 (t, *J* = 7.5 Hz, 2H), 6.46 (t, *J* = 7.4 Hz, 1H) ppm. **^{13}C NMR (125 MHz, CDCl$_3$)** δ 141.9, 140.9 (2C), 140.6, 140.5, 139.9, 139.0, 138.7, 137.8, 133.6, 131.9, 131.3 (2C), 131.2, 131.1, 128.3, 127.5, 126.5, 126.4, 126.2, 125.2, 125.1, 125.0 (2C), 124.6, 124.4 (2C), 119.7, 117.5, 112.9 ppm. **HRMS (ESI-TOF) m/z:** [M + H]$^+$ Calcd for $C_{41}H_{27}ClN_2$ 583.1941, found 583.1955.

6-Fluoro-2-(5,6,7,8-tetraphenylnaphthalen-1-yl)imidazo[1,2-*a*]pyridine (5e)



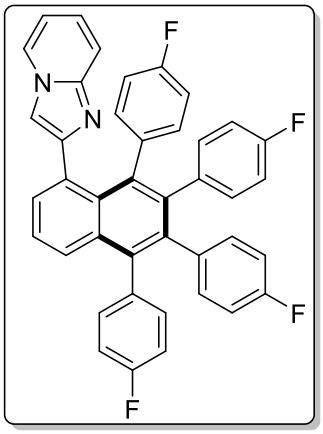
Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 206-210 ºC, yield: (111 mg, 76%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.71 (dd, *J* = 8.5, 0.8 Hz, 1H), 7.67 – 7.64 (m, 1H), 7.58 – 7.53 (m, 1H), 7.42 (dd, *J* = 8.3, 7.1 Hz, 1H), 7.31 (dd, *J* = 9.7, 5.1 Hz, 1H), 7.25 – 7.21 (m, 4H), 7.21 – 7.17 (m, 1H), 6.97 (dd, *J* = 12.8, 5.1 Hz, 1H), 6.89 – 6.77 (m, 8H), 6.76 – 6.70 (m, 3H), 6.67 (dd, *J* = 6.9, 2.3 Hz, 2H), 6.53 (t, *J* = 7.5 Hz, 2H), 6.45 (t, *J* = 7.4 Hz, 1H) ppm. **^{13}C NMR (125 MHz, $CDCl_3$)** δ 153.0 (d, J_{CF} = 236.8 Hz), 148.2 (2C), 141.2, 141.0, 140.9, 140.6 (d, J_{CF} = 3.7 Hz), 139.9, 139.0, 138.7, 137.8, 133.6, 131.9, 131.3 (2C), 131.2, 131.1, 128.3, 127.5, 126.5, 126.4, 126.2, 125.2, 125.1, 125.0, 124.9, 124.3, 117.4 (d, J_{CF} = 8.8 Hz), 115.5 (d, J_{CF} = 20.1 Hz), 113.9, 111.3, 111.0 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{41}H_{27}FN_2$ 567.2237, found 567.2240.**^{19}F NMR (471 MHz, $CDCl_3$)** δ -141.63 (s) ppm.

2-(5,6,7,8-Tetrakis(4-chlorophenyl)naphthalen-1-yl)imidazo[1,2-*a*]pyridine (5g)



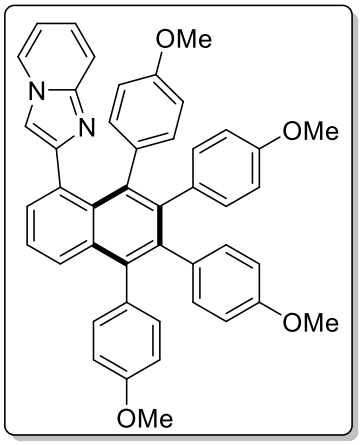
Yellow solid, eluent: (hexane/EtOAc, 95:5), m.p. 268-270 ºC, yield: (145 mg, 77%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.85 (d, *J* = 6.6 Hz, 1H), 7.64 – 7.57 (m, 2H), 7.48 – 7.43 (m, 1H), 7.37 – 7.34 (m, 1H), 7.28 – 7.25 (m, 3H), 7.14 – 11 (m, 3H), 6.93 – 6.88 (m, 3H), 6.80 (d, *J* = 8.4 Hz, 2H), 6.70 – 6.67 (m, 5H), 6.59 – 6.51 (m, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 147.0, 143.8, 139.4, 139.1, 138.5, 138.0, 137.9, 137.6, 133.6, 133.3, 132.9, 132.5, 132.3, 132.1, 139.1, 131.7, 131.4, 131.2, 128.1, 127.8, 127.2, 126.9, 125.4, 125.3, 124.8, 124.3, 117.1, 112.3, 111.8 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{41}H_{24}Cl_4N_2$ 685.0772, found 685.0771.

2-(5,6,7,8-Tetrakis(4-fluorophenyl)naphthalen-1-yl)imidazo[1,2-*a*]pyridine (5h)



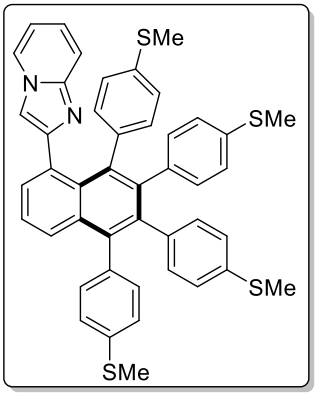
White solid, eluent: (hexane/EtOAc, 95:5), m.p. 186-188 ^{o}C, yield: (122 mg, 72%). **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.75 (d, *J* = 6.8 Hz, 1H), 7.59 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.50 (dd, *J* = 6.9, 1.3 Hz, 1H), 7.37 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.29 (d, *J* = 9.0 Hz, 1H), 7.19 (s, 1H), 7.10 – 7.06 (m, 2H), 7.05 – 7.01 (m, 1H), 6.92 – 6.87 (m, 3H), 6.63 (ddd, *J* = 7.1, 4.4, 2.0 Hz, 4H), 6.54 – 6.49 (m, 4H), 6.42 (t, *J* = 8.8 Hz, 2H), 6.17 (t, *J* = 8.8 Hz, 2H) ppm. **^{13}C NMR (75 MHz, CDCl$_3$)** δ 161.6 (d, J_{CF} = 245.2 Hz), 160.7 (d, J_{CF} = 244.5 Hz), 160.6 (d, J_{CF} = 243.0 Hz), 160.4 (d, J_{CF} = 243.7 Hz), 147.2, 143.8, 140.0, 138.2 (d, J_{CF} = 3.7 Hz), 137.7, 136.7 (d, J_{CF} = 3.7 Hz), 136.3 (2C), 136.2, 135.6 (d, J_{CF} = 3.7 Hz), 133.8, 133.3, 133.2, 133.1, 132.8, 132.7, 132.6, 132.5, 132.4, 132.3, 131.5, 127.8, 125.0, 124.6, 124.1, 117.1, 114.7 (d, J_{CF} = 21.7 Hz), 113.9, 113.7, 113.6, 113.4, 112.1, 112.0, 111.8 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{41}H_{24}F_4N_2$ 621.1954, found 621.1915.**^{19}F NMR (471 MHz, CDCl$_3$)** δ -115.47 (s), -116.57 (s), -116.92 (s), -117.56 (s) ppm.

2-(5,6,7,8-Tetrakis(4-methoxyphenyl)naphthalen-1-yl)imidazo[1,2-*a*]pyridine (5i)



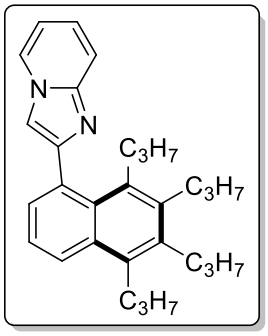
Brown solid, eluent: (hexane/EtOAc, 80:20), m.p. 140-142 ^{o}C, yield: (125 mg, 68%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.69 (d, *J* = 6.8 Hz, 1H), 7.64 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.49 (dd, *J* = 6.9, 1.3 Hz, 1H), 7.33 – 7.30 (m, 1H), 7.19 (s, 2H), 7.04 (d, *J* = 8.7 Hz, 3H), 6.76 – 6.72 (m, 3H), 6.60 (d, *J* = 8.7 Hz, 4H), 6.48 (d, *J* = 8.8 Hz, 2H), 6.34 (d, *J* = 8.8 Hz, 2H), 6.26 (d, *J* = 8.8 Hz, 2H), 6.01 (d, *J* = 8.7 Hz, 2H), 3.73 (s, 3H), 3.55 (s, 3H), 3.50 (s, 3H), 3.27 (s, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 157.9, 156.7, 147.3, 143.4, 140.9, 139.2, 138.4, 137.7, 133.9, 133.5, 133.4, 132.8, 132.6, 132.3, 132.2, 132.0, 131.5, 131.1, 128.0, 124.5, 124.2, 123.3, 117.0, 113.5, 113.0, 112.3, 112.1, 111.8, 111.5, 110.8, 55.1, 55.0, 54.8, 54.6 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{45}H_{36}N_2O_4$ 669.2753, found 669.2719.

2-(5,6,7,8-Tetrakis(4-(methylthio)phenyl)naphthalen-1-yl)imidazo[1,2-*a*]pyridine (5j)



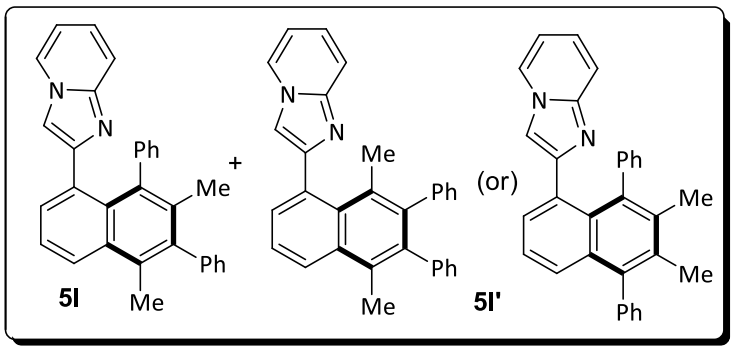
Yellow solid, eluent: (hexane/EtOAc, 90:10), m.p. 196-198 ^{o}C, yield: (141 mg, 70%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.77 (d, *J* = 6.7 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.49 (dd, *J* = 6.9, 1.1 Hz, 1H), 7.34 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.19 (s, 1H), 7.06 (dd, *J* = 18.2, 8.4 Hz, 6H), 6.80 (s, 1H), 6.70 (d, *J* = 8.4 Hz, 2H), 6.65 – 6.59 (m, 6H), 6.49 (d, *J* = 8.3 Hz, 2H), 6.38 (d, *J* = 8.3 Hz, 2H), 2.41 (s, 3H), 2.24 (s, 3H), 2.19 (s, 3H), 2.00 (s, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 143.1, 140.4, 138.5, 138.4, 138.0, 137.5, 136.7 (2C), 135.2, 135.0, 134.9, 133.8, 132.2, 132.0, 131.8, 131.7, 131.5, 131.4, 131.3, 128.5, 128.3, 126.0, 125.6, 125.4, 125.3, 124.8, 124.5, 124.1, 116.8, 112.4, 112.2, 16.1, 15.9 (2C), 15.8 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{45}H_{36}N_2S_4$ 733.1840, found 733.1787.

2-(5,6,7,8-Tetrapropylnaphthalen-1-yl)imidazo[1,2-*a*]pyridine (5k)



Brown oil, eluent: (hexane/EtOAc, 97:3), yield: (85 mg, 52%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 8.05 (d, *J* = 6.6 Hz, 1H), 7.99 – 7.96 (m, 1H), 7.54 (d, *J* = 9.0 Hz, 1H), 7.49 (s, 1H), 7.28 – 7.26 (m, 2H), 7.09 (t, *J* = 7.8 Hz, 1H), 6.71 (t, *J* = 6.9 Hz, 1H), 3.0 – 2.94 (m, 2H), 2.69 – 2.58 (m, 4H), 2.39 – 2.33 (m, 2H), 1.67 – 1.43 (m, 8H), 1.06 – 1.02 (m, 6H), 0.99 – 0.93 (m, 3H), 6.31 (t, *J* = 7.2 Hz, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 150.3, 144.3, 138.7, 137.0, 135.7, 134.1, 132.6, 131.6, 130.8, 130.3, 125.3, 125.1, 124.1, 122.8, 117.6, 112.1, 110.1, 32.8, 32.7, 32.3, 31.7, 25.3, 24.9, 24.7, 24.5, 14.9, 14.8, 14.7, 14.0 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{29}H_{36}N_2$ 413.2957, found 413.2963.

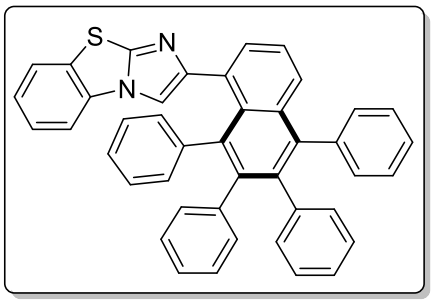
2-(5,7-dimethyl-6,8-diphenylnaphthalen-1-yl)imidazo[1,2-a]pyridine (5l) and 2-(5,8-dimethyl-6,7-diphenylnaphthalen-1-yl)imidazo[1,2-a]pyridine (5l')



Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 118-120 ºC, yield: (72 mg, 62%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.16 – 8.14 (m, 1H), 8.08 – 8.04 (m, 2H), 7.90-7.88 (m, 1H), 7.79 (s, 0.6 H), 7.59-7.55 (m, 5H), 7.51-7.47 (m, 1H), 7.44-7.41 (m, 2.5), 7.39-7.30 (m, 4.5H), 7.28-7.20 (m, 2H), 7.18 (s, 1H), 7.16-7.15 (m, 2H), 7.12-7.09 (m, 2.6H), 7.07-7.04 (m, 2H), 7.01-6.97 (m, 3H), 6.93-6.88 (m, 5H), 6.74-6.71 (m, 2H), 2.40 (s, 3H), 2.42 (s, 3H), 1.76 (s, 3H), 1.75 (s, 3H), 1.73 (s, 3H) ppm. **^{13}C NMR (125 MHz, $CDCl_3$)** δ 162.6, 161.6, 161.5 (2C), 160.6, 159.7, 159.5 (2C), 148.2, 147.0, 146.3, 140.1, 138.2 (2C), 137.6, 136.8 (2C), 136.3, 136.2 (3C), 135.5

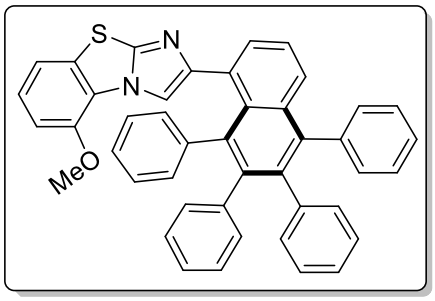
(2C), 133.8, 133.3, 133.2, 132.7 (2C), 132.5 (2C), 132.3 (2C), 131.8, 131.5, 131.4, 129.8, 128.0, 126.0, 125.1, 124.6, 124.3, 114.8, 114.7, 113.9, 113.8, 113.7, 113.5, 112.1, 112.1, 112.0, 110.2, 31.4, 30.1, 29.6 (2C) ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{31}H_{24}N_2$ 425.2018, found 425.2019.

2-(5,6,7,8-Tetraphenylnaphthalen-1-yl)benzo[*d*]imidazo[2,1-*b*]thiazole (7a)



Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 236-238 °C, yield: (100 mg, 73%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.73 – 7.70 (m, 1H), 7.65 – 7.63 (m, 2H), 7.45 – 7.22 (m, 9H), 6.96 – 6.94 (m, 2H), 6.87 – 6.80 (m, 7H), 6.75 – 6.58 (m, 2H), 6.55 – 6.34 (m, 1H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 148.3, 145.8, 141.2, 140.9, 140.7, 140.0, 139.0, 138.7, 138.1, 133.7, 132.9, 132.0, 131.4, 131.2, 131.1, 130.0, 128.1, 127.7, 127.6, 127.4, 126.4, 126.3, 126.1, 125.7, 125.1, 125.0, 124.9, 124.6, 124.2, 124.1, 124.0, 112.1, 110.7 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{43}H_{28}N_2S$ 605.2051, found 605.2051.

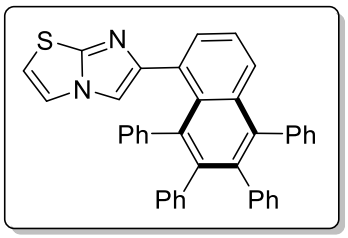
5-Methoxy-2-(5,6,7,8-tetraphenylnaphthalen-1-yl)benzo[*d*]imidazo[2,1-*b*]thiazole (7b)



Brown solid, eluent: (hexane/EtOAc, 90:10), m.p. 194-197 °C, yield: (79 mg, 60%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.71 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.64 (d, *J* = 6.8 Hz, 1H), 7.44 (dd, *J* = 8.4, 7.0 Hz, 1H), 7.32 (s, 1H), 7.27 (dd, *J* = 5.2, 4.1 Hz, 4H), 7.25 – 7.19 (m, 3H), 6.91 (dd, *J* = 6.4, 2.5 Hz, 1H), 6.89 – 6.81 (m, 7H), 6.81 – 6.75 (m, 3H), 6.75 – 6.69 (m, 2H), 6.58 (t, *J* = 7.7 Hz, 2H), 6.36 (t, *J* = 7.4 Hz, 1H), 4.00 (s, 3H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 147.5, 147.3, 145.0, 141.2, 140.8, 140.2, 138.9, 138.7, 138.2, 133.7, 133.3, 132.0, 131.4, 131.2 (2C), 127.9,

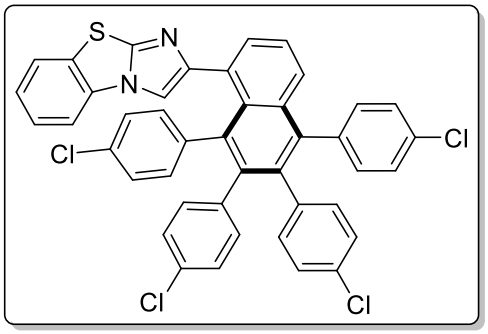
127.4, 126.6, 126.4, 126.3, 126.1, 125.1, 125.0, 124.8, 124.6, 124.4, 124.0, 122.4, 115.9, 114.9, 113.4, 107.8, 56.0 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{44}H_{30}N_2OS$ 635.2157, found 635.2123.

6-(5,6,7,8-Tetraphenylnaphthalen-1-yl)imidazo[2,1-*b*]thiazole (7c)



Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 138-142 ºC, yield: (97 mg, 65%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.68 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.53 (dd, *J* = 6.9, 1.3 Hz, 1H), 7.40 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.25 – 7.20 (m, 4H), 7.19 – 7.16 (m, 1H), 7.04 (d, *J* = 4.5 Hz, 1H), 6.81 (ddd, *J* = 19.3, 9.5, 6.2 Hz, 7H), 6.75 (td, *J* = 4.7, 2.3 Hz, 4H), 6.70 – 6.67 (m, 2H), 6.66 – 6.56 (m, 4H) ppm. **^{13}C NMR (125 MHz, $CDCl_3$)** δ 141.15, 140.84, 140.72, 140.06, 138.92, 138.63, 138.11, 133.65, 133.12, 132.06, 131.40, 131.39, 131.30, 131.13, 128.10, 127.50, 126.47, 126.39, 126.16, 125.20, 124.90, 124.65, 124.10, 117.84, 111.66, 111.28 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{39}H_{26}N_2S$ 555.1895, found 555.1904.

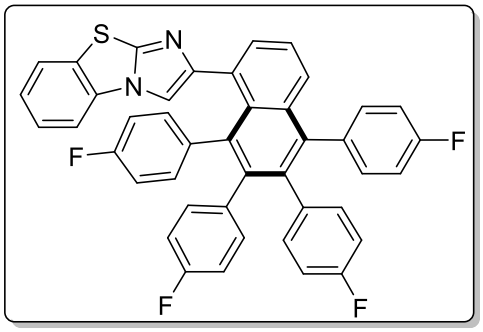
2-(5,6,7,8-Tetrakis(4-chlorophenyl)naphthalen-1-yl)benzo[*d*]imidazo[2,1-*b*]thiazole (7d)



Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 288-290 ºC, yield: (115 mg, 68%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.70 – 7.67 (m, 1H), 7.65 – 7.60 (m, 2H), 7.49 – 7.46 (m, 1H), 7.44 – 7.39 (m, 2H), 7.36 – 7.33 (m, 1H), 7.31 – 7.26 (m, 3H), 7.14 – 7.11 (m, 2H), 7.02 (s, 1H), 6.91 – 6.88 (m, 2H), 6.82 – 6.79 (m, 2H), 6.76 – 6.68 (m, 3H), 6.61 – 6.60 (m, 2H), 6.59 – 6.58 (m, 1H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 148.0, 146.5, 139.4, 139.0, 138.5, 138.1, 137.9, 137.5 (2C), 133.6, 133.0, 132.9, 132.4, 132.3, 132.1, 131.9 (2C), 131.7, 131.6, 131.3, 131.1, 130.0, 128.0,

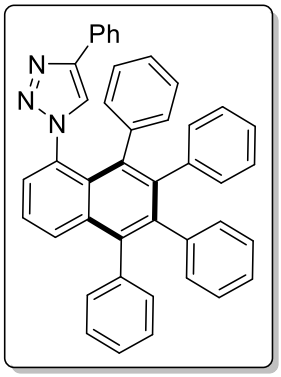
127.9, 127.2, 126.9, 126.0, 125.4, 125.3, 124.6, 124.2, 112.2, 110.5 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{43}H_{24}Cl_4N_2S$ 741.0493, found 741.0460.

2-(5,6,7,8-Tetrakis(4-fluorophenyl)naphthalen-1-yl)benzo[*d*]imidazo[2,1-*b*]thiazole (7e)



Brown solid, eluent: (hexane/EtOAc, 95:5), m.p. 216-219 ^oC, yield: (100 mg, 65%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.70 – 7.62 (m, 2H), 7.59 (dd, *J* = 6.9, 1.1 Hz, 1H), 7.45 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.38 – 7.34 (m, 1H), 7.34 – 7.29 (m, 1H), 7.14 (td, *J* = 8.8, 5.9 Hz, 2H), 7.05 (s, 1H), 6.97 (t, *J* = 8.7 Hz, 2H), 6.77 (dd, *J* = 8.5, 5.6 Hz, 2H), 6.73 – 6.66 (m, 2H), 6.59 (ddd, *J* = 11.6, 7.0, 4.7 Hz, 4H), 6.50 (t, *J* = 8.7 Hz, 2H), 6.32 (t, *J* = 8.7 Hz, 2H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 161.6 (d, J_{CF} = 245.2 Hz), 160.7 (d, J_{CF} = 243.7 Hz), 160.6 (d, J_{CF} = 243.7 Hz) (2C), 148.1, 146.3, 140.2, 138.3 (d, J_{CF} = 2.8 Hz), 137.6, 136.8 (d, J_{CF} = 3.4 Hz), 136.3, 136.2 (2C), 135.5 (d, J_{CF} = 5.2 Hz), 133.3 (d, J_{CF} = 7.8 Hz), 132.7, 132.6 (2C), 132.5, 132.4, 132.3, 131.9, 131.6, 129.9, 128.1, 126.0, 125.1, 124.4 (d, J_{CF} = 28.2 Hz), 114.7 (d, J_{CF} = 21.2 Hz), 113.9, 113.7, 113.4, 112.2, 112.0, 111.9, 110.2 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{43}H_{24}F_4N_2S$ 677.1675, found 677.1641.**^{19}F NMR (471 MHz, $CDCl_3$)** δ -115.44 (s), -116.54 (s), -116.87 (s), -117.50 (s) ppm.

4-Phenyl-1-(5,6,7,8-tetraphenylnaphthalen-1-yl)-1*H*-1,2,3-triazole (9a)



Yellow solid, eluent: (hexane/EtOAc, 95:5), m.p. 214-218 ^{o}C, yield: (112 mg, 78%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.92 (dd, J = 6.3 Hz, J = 3.0 Hz, 1H), 7.58 – 7.53 (m, 2H), 7.50 – 7.48 (m, 2H), 7.40 – 7.27 (m, 9H), 6.68 – 6.85 (m, 7H), 6.78 – 6.68 (m, 7H), 6.62 – 6.59 (m, 1H) ppm. **^{13}C NMR (75 MHz, $CDCl_3$)** δ 146.8, 142.9, 140.3, 140.0, 139.8, 139.3, 139.1, 138.9, 135.9, 134.2, 134.1, 131.2, 131.0, 130.9, 130.7, 130.6, 130.5, 128.5, 127.9, 127.7, 127.6, 127.5, 126.8, 126.6, 126.3, 125.8 (2C), 125.5, 125.3, 124.7, 123.8 ppm. **HRMS (ESI-TOF) m/z:** $[M + H]^+$ Calcd for $C_{42}H_{29}N_3$ 576.2440, found 576.2446.

Table S1. Crystal data and structure refinement for **3k**.

Identification code	KP-TS-526	
CCDC Number	2143782	
Empirical formula	C_{27} H_{22} N_2	
Formula weight	374.46	
Temperature	297(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.0767(4) Å	a= 90°.
	b = 7.7890(2) Å	b= 101.9960(10)°.
	c = 22.3524(6) Å	g = 90°.
Volume	2056.67(10) $Å^3$	
Z	4	
Density (calculated)	1.209 Mg/m^3	
Absorption coefficient	0.542 mm^{-1}	
F(000)	792	
Crystal size	0.320 x 0.260 x 0.170 mm^3	
Theta range for data collection	3.866 to 70.148°.	
Index ranges	-14<=h<=14, -9<=k<=9, -27<=l<=27	
Reflections collected	48923	
Independent reflections	3887 [R(int) = 0.0586]	
Completeness to theta = 67.679°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.753 and 0.594	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3887 / 0 / 263	
Goodness-of-fit on F^2	0.881	
Final R indices [I>2sigma(I)]	R1 = 0.0623, wR2 = 0.2130	
R indices (all data)	R1 = 0.0675, wR2 = 0.2269	
Extinction coefficient	0.008(2)	
Largest diff. peak and hole	0.261 and -0.278 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 526_sx. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4846(1)	3698(2)	1902(1)	61(1)
C(2)	3978(1)	2860(2)	1508(1)	59(1)
C(3)	3521(1)	1308(2)	1703(1)	59(1)
C(4)	2530(2)	457(2)	1371(1)	66(1)
C(5)	2197(2)	-1104(3)	1549(1)	77(1)
C(6)	2798(2)	-1905(3)	2071(1)	82(1)
C(7)	3695(2)	-1086(2)	2431(1)	75(1)
C(8)	4070(1)	537(2)	2267(1)	62(1)
C(9)	4973(2)	1423(2)	2665(1)	64(1)
C(10)	5315(1)	2993(2)	2490(1)	61(1)
C(11)	6228(1)	3981(2)	2911(1)	62(1)
C(12)	7363(2)	3719(3)	2906(1)	74(1)
C(13)	8194(2)	4654(3)	3293(1)	83(1)
C(14)	7898(2)	5840(3)	3689(1)	83(1)
C(15)	6771(2)	6112(3)	3696(1)	81(1)
C(16)	5945(2)	5184(2)	3310(1)	71(1)
C(17)	5524(2)	623(3)	3264(1)	87(1)
C(18)	3629(1)	3517(2)	865(1)	63(1)
C(19)	4031(2)	2691(3)	401(1)	78(1)
C(20)	3791(2)	3343(4)	-192(1)	97(1)
C(21)	3167(2)	4798(4)	-329(1)	100(1)
C(22)	2768(2)	5623(3)	120(1)	100(1)
C(23)	2998(2)	4981(3)	717(1)	82(1)
C(24)	5358(2)	5329(3)	1716(1)	77(1)
C(25)	1614(2)	947(3)	269(1)	90(1)
C(26)	770(2)	2004(4)	-16(1)	105(1)
C(27)	461(2)	2923(4)	447(1)	100(1)
N(1)	1781(1)	1285(2)	872(1)	71(1)
N(2)	1064(1)	2508(3)	992(1)	87(1)

Table S4. Bond lengths [Å] and angles [°] for **3k**.

C(1)-C(2)	1.384(2)
C(1)-C(10)	1.429(2)
C(1)-C(24)	1.509(2)
C(2)-C(3)	1.434(2)
C(2)-C(18)	1.501(2)
C(3)-C(8)	1.430(2)
C(3)-C(4)	1.432(2)
C(4)-C(5)	1.366(3)
C(4)-N(1)	1.436(2)
C(5)-C(6)	1.387(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.366(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.416(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.433(3)
C(9)-C(10)	1.374(2)
C(9)-C(17)	1.501(3)
C(10)-C(11)	1.504(2)
C(11)-C(16)	1.385(3)
C(11)-C(12)	1.388(3)
C(12)-C(13)	1.387(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.378(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.381(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.381(3)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(23)	1.373(3)

C(18)-C(19)	1.390(3)
C(19)-C(20)	1.393(3)
C(19)-H(19)	0.9300
C(20)-C(21)	1.360(4)
C(20)-H(20)	0.9300
C(21)-C(22)	1.361(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.396(3)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-N(1)	1.347(3)
C(25)-C(26)	1.361(4)
C(25)-H(25)	0.9300
C(26)-C(27)	1.373(4)
C(26)-H(26)	0.9300
C(27)-N(2)	1.322(3)
C(27)-H(27)	0.9300
N(1)-N(2)	1.350(3)
C(2)-C(1)-C(10)	120.46(15)
C(2)-C(1)-C(24)	121.49(15)
C(10)-C(1)-C(24)	118.00(15)
C(1)-C(2)-C(3)	119.52(15)
C(1)-C(2)-C(18)	118.21(14)
C(3)-C(2)-C(18)	121.96(14)
C(8)-C(3)-C(4)	116.50(15)
C(8)-C(3)-C(2)	119.05(14)
C(4)-C(3)-C(2)	124.45(15)
C(5)-C(4)-C(3)	121.76(17)
C(5)-C(4)-N(1)	116.75(16)
C(3)-C(4)-N(1)	121.20(16)
C(4)-C(5)-C(6)	120.70(18)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6

C(7)-C(6)-C(5)	119.87(18)
C(7)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
C(6)-C(7)-C(8)	121.40(19)
C(6)-C(7)-H(7)	119.3
C(8)-C(7)-H(7)	119.3
C(7)-C(8)-C(3)	119.28(16)
C(7)-C(8)-C(9)	120.81(16)
C(3)-C(8)-C(9)	119.89(15)
C(10)-C(9)-C(8)	119.16(15)
C(10)-C(9)-C(17)	121.30(16)
C(8)-C(9)-C(17)	119.54(16)
C(9)-C(10)-C(1)	121.27(15)
C(9)-C(10)-C(11)	120.16(15)
C(1)-C(10)-C(11)	118.54(15)
C(16)-C(11)-C(12)	118.72(16)
C(16)-C(11)-C(10)	120.10(15)
C(12)-C(11)-C(10)	121.18(16)
C(13)-C(12)-C(11)	120.40(19)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(14)-C(13)-C(12)	120.17(19)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-C(15)	119.85(19)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(16)-C(15)-C(14)	120.0(2)
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(15)-C(16)-C(11)	120.90(18)
C(15)-C(16)-H(16)	119.6
C(11)-C(16)-H(16)	119.5
C(9)-C(17)-H(17A)	109.5
C(9)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5

C(9)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(23)-C(18)-C(19)	117.80(18)
C(23)-C(18)-C(2)	123.05(17)
C(19)-C(18)-C(2)	118.96(17)
C(18)-C(19)-C(20)	120.4(2)
C(18)-C(19)-H(19)	119.8
C(20)-C(19)-H(19)	119.8
C(21)-C(20)-C(19)	120.9(2)
C(21)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(20)-C(21)-C(22)	119.5(2)
C(20)-C(21)-H(21)	120.3
C(22)-C(21)-H(21)	120.3
C(21)-C(22)-C(23)	120.3(2)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(18)-C(23)-C(22)	121.2(2)
C(18)-C(23)-H(23)	119.4
C(22)-C(23)-H(23)	119.4
C(1)-C(24)-H(24A)	109.5
C(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(1)-C(25)-C(26)	107.0(2)
N(1)-C(25)-H(25)	126.5
C(26)-C(25)-H(25)	126.5
C(25)-C(26)-C(27)	104.9(2)
C(25)-C(26)-H(26)	127.6
C(27)-C(26)-H(26)	127.6
N(2)-C(27)-C(26)	112.5(2)
N(2)-C(27)-H(27)	123.7
C(26)-C(27)-H(27)	123.7

C(25)-N(1)-N(2)	111.53(18)
C(25)-N(1)-C(4)	129.01(19)
N(2)-N(1)-C(4)	119.29(15)
C(27)-N(2)-N(1)	104.1(2)

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 526_sx. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	61(1)	64(1)	56(1)	2(1)	9(1)	-2(1)
C(2)	59(1)	62(1)	57(1)	1(1)	10(1)	-1(1)
C(3)	59(1)	62(1)	57(1)	-2(1)	14(1)	0(1)
C(4)	63(1)	70(1)	66(1)	-5(1)	16(1)	-5(1)
C(5)	73(1)	74(1)	86(1)	-6(1)	20(1)	-14(1)
C(6)	87(1)	69(1)	92(1)	5(1)	26(1)	-15(1)
C(7)	84(1)	68(1)	74(1)	9(1)	21(1)	0(1)
C(8)	65(1)	62(1)	62(1)	1(1)	17(1)	2(1)
C(9)	67(1)	66(1)	58(1)	3(1)	11(1)	5(1)
C(10)	61(1)	66(1)	57(1)	-1(1)	9(1)	2(1)
C(11)	60(1)	67(1)	56(1)	4(1)	5(1)	2(1)
C(12)	65(1)	83(1)	72(1)	-3(1)	10(1)	5(1)
C(13)	59(1)	97(1)	88(1)	6(1)	2(1)	-2(1)
C(14)	77(1)	82(1)	79(1)	0(1)	-7(1)	-11(1)
C(15)	87(1)	77(1)	72(1)	-12(1)	3(1)	1(1)
C(16)	67(1)	77(1)	67(1)	-4(1)	10(1)	3(1)
C(17)	95(1)	83(1)	74(1)	17(1)	-1(1)	-4(1)
C(18)	61(1)	69(1)	57(1)	3(1)	5(1)	-9(1)
C(19)	78(1)	94(1)	62(1)	0(1)	14(1)	-5(1)
C(20)	97(2)	131(2)	64(1)	3(1)	20(1)	-16(2)
C(21)	97(2)	125(2)	70(1)	26(1)	-2(1)	-21(2)
C(22)	102(2)	90(2)	94(2)	28(1)	-12(1)	-3(1)
C(23)	86(1)	78(1)	74(1)	5(1)	0(1)	3(1)
C(24)	79(1)	79(1)	68(1)	11(1)	3(1)	-18(1)
C(25)	96(2)	103(2)	68(1)	-14(1)	9(1)	-27(1)
C(26)	94(2)	134(2)	75(1)	14(1)	-13(1)	-38(2)
C(27)	69(1)	133(2)	93(2)	28(2)	5(1)	-2(1)
N(1)	62(1)	83(1)	65(1)	-4(1)	7(1)	-11(1)
N(2)	68(1)	110(1)	82(1)	12(1)	15(1)	12(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **3k.**

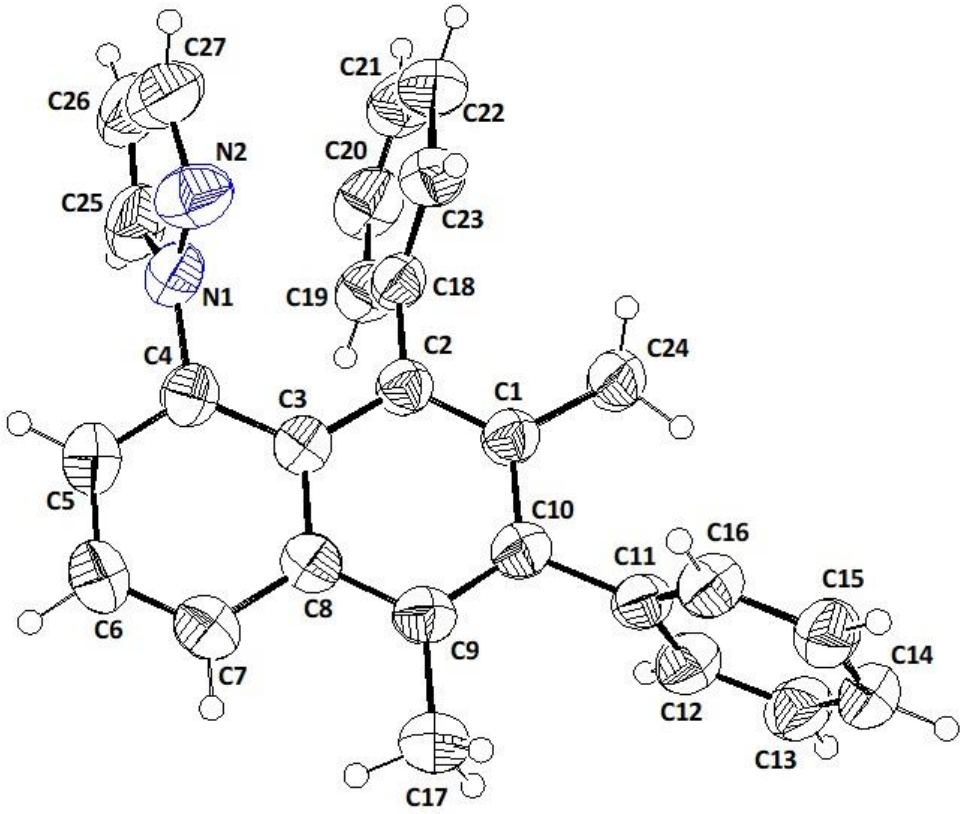
	x	y	z	U(eq)
H(5)	1559	-1636	1318	93
H(6)	2591	-2997	2175	98
H(7)	4067	-1605	2792	89
H(12)	7568	2913	2642	89
H(13)	8952	4479	3285	100
H(14)	8457	6456	3952	99
H(15)	6569	6921	3960	97
H(16)	5187	5369	3318	85
H(17A)	5176	-465	3307	130
H(17B)	6316	457	3274	130
H(17C)	5434	1366	3593	130
H(19)	4462	1698	488	94
H(20)	4062	2776	-498	116
H(21)	3014	5226	-726	120
H(22)	2341	6618	30	120
H(23)	2719	5555	1019	98
H(24A)	5944	5718	2047	116
H(24B)	5674	5111	1363	116
H(24C)	4783	6194	1620	116
H(25)	2001	144	82	108
H(26)	468	2085	-434	127
H(27)	-109	3747	385	120

Table S7. Torsion angles [°] for **3k**.

C(10)-C(1)-C(2)-C(3)	2.4(2)
C(24)-C(1)-C(2)-C(3)	179.64(16)
C(10)-C(1)-C(2)-C(18)	-171.43(15)
C(24)-C(1)-C(2)-C(18)	5.8(3)
C(1)-C(2)-C(3)-C(8)	-8.2(2)
C(18)-C(2)-C(3)-C(8)	165.32(16)
C(1)-C(2)-C(3)-C(4)	171.26(16)
C(18)-C(2)-C(3)-C(4)	-15.2(3)
C(8)-C(3)-C(4)-C(5)	-6.9(3)
C(2)-C(3)-C(4)-C(5)	173.62(17)
C(8)-C(3)-C(4)-N(1)	166.83(15)
C(2)-C(3)-C(4)-N(1)	-12.7(3)
C(3)-C(4)-C(5)-C(6)	1.6(3)
N(1)-C(4)-C(5)-C(6)	-172.42(18)
C(4)-C(5)-C(6)-C(7)	3.8(3)
C(5)-C(6)-C(7)-C(8)	-3.5(3)
C(6)-C(7)-C(8)-C(3)	-2.1(3)
C(6)-C(7)-C(8)-C(9)	176.67(19)
C(4)-C(3)-C(8)-C(7)	7.0(2)
C(2)-C(3)-C(8)-C(7)	-173.47(15)
C(4)-C(3)-C(8)-C(9)	-171.73(15)
C(2)-C(3)-C(8)-C(9)	7.8(2)
C(7)-C(8)-C(9)-C(10)	179.89(16)
C(3)-C(8)-C(9)-C(10)	-1.4(3)
C(7)-C(8)-C(9)-C(17)	-0.2(3)
C(3)-C(8)-C(9)-C(17)	178.47(17)
C(8)-C(9)-C(10)-C(1)	-4.7(3)
C(17)-C(9)-C(10)-C(1)	175.48(18)
C(8)-C(9)-C(10)-C(11)	177.50(15)
C(17)-C(9)-C(10)-C(11)	-2.4(3)
C(2)-C(1)-C(10)-C(9)	4.2(3)
C(24)-C(1)-C(10)-C(9)	-173.13(17)
C(2)-C(1)-C(10)-C(11)	-177.88(15)
C(24)-C(1)-C(10)-C(11)	4.7(2)

C(9)-C(10)-C(11)-C(16)	-92.9(2)
C(1)-C(10)-C(11)-C(16)	89.2(2)
C(9)-C(10)-C(11)-C(12)	87.5(2)
C(1)-C(10)-C(11)-C(12)	-90.4(2)
C(16)-C(11)-C(12)-C(13)	-0.3(3)
C(10)-C(11)-C(12)-C(13)	179.37(18)
C(11)-C(12)-C(13)-C(14)	0.6(3)
C(12)-C(13)-C(14)-C(15)	-0.7(3)
C(13)-C(14)-C(15)-C(16)	0.6(3)
C(14)-C(15)-C(16)-C(11)	-0.3(3)
C(12)-C(11)-C(16)-C(15)	0.2(3)
C(10)-C(11)-C(16)-C(15)	-179.50(17)
C(1)-C(2)-C(18)-C(23)	-75.3(2)
C(3)-C(2)-C(18)-C(23)	111.1(2)
C(1)-C(2)-C(18)-C(19)	99.6(2)
C(3)-C(2)-C(18)-C(19)	-74.1(2)
C(23)-C(18)-C(19)-C(20)	-0.1(3)
C(2)-C(18)-C(19)-C(20)	-175.27(18)
C(18)-C(19)-C(20)-C(21)	0.3(4)
C(19)-C(20)-C(21)-C(22)	-0.3(4)
C(20)-C(21)-C(22)-C(23)	0.0(4)
C(19)-C(18)-C(23)-C(22)	-0.1(3)
C(2)-C(18)-C(23)-C(22)	174.83(19)
C(21)-C(22)-C(23)-C(18)	0.1(4)
N(1)-C(25)-C(26)-C(27)	-0.8(3)
C(25)-C(26)-C(27)-N(2)	0.5(3)
C(26)-C(25)-N(1)-N(2)	0.9(2)
C(26)-C(25)-N(1)-C(4)	176.19(19)
C(5)-C(4)-N(1)-C(25)	-76.9(3)
C(3)-C(4)-N(1)-C(25)	109.1(2)
C(5)-C(4)-N(1)-N(2)	98.1(2)
C(3)-C(4)-N(1)-N(2)	-75.9(2)
C(26)-C(27)-N(2)-N(1)	0.1(3)
C(25)-N(1)-N(2)-C(27)	-0.6(2)
C(4)-N(1)-N(2)-C(27)	-176.38(17)

ORTEP crystal structure of compound **3k**



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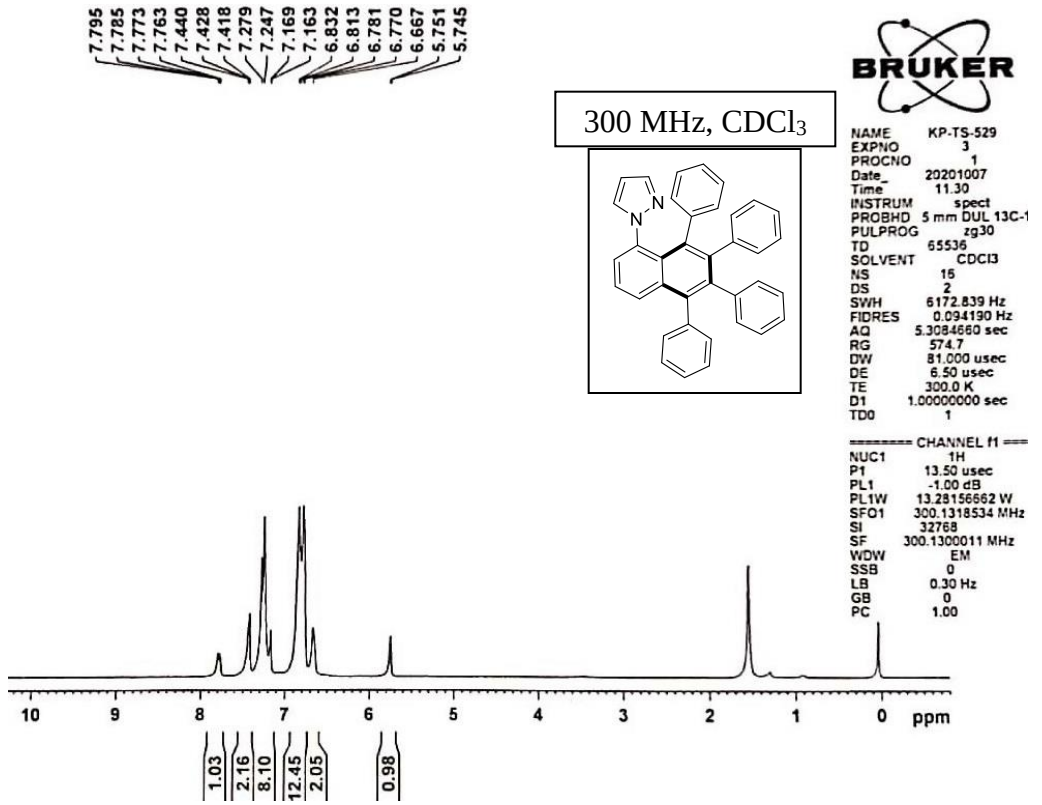
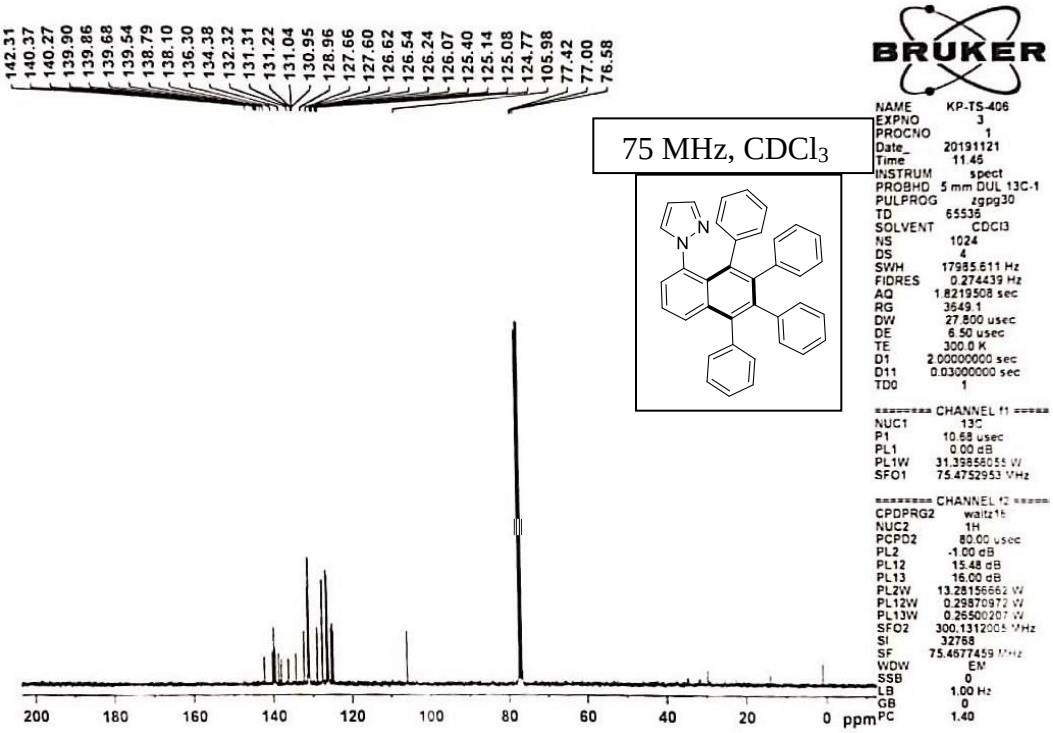
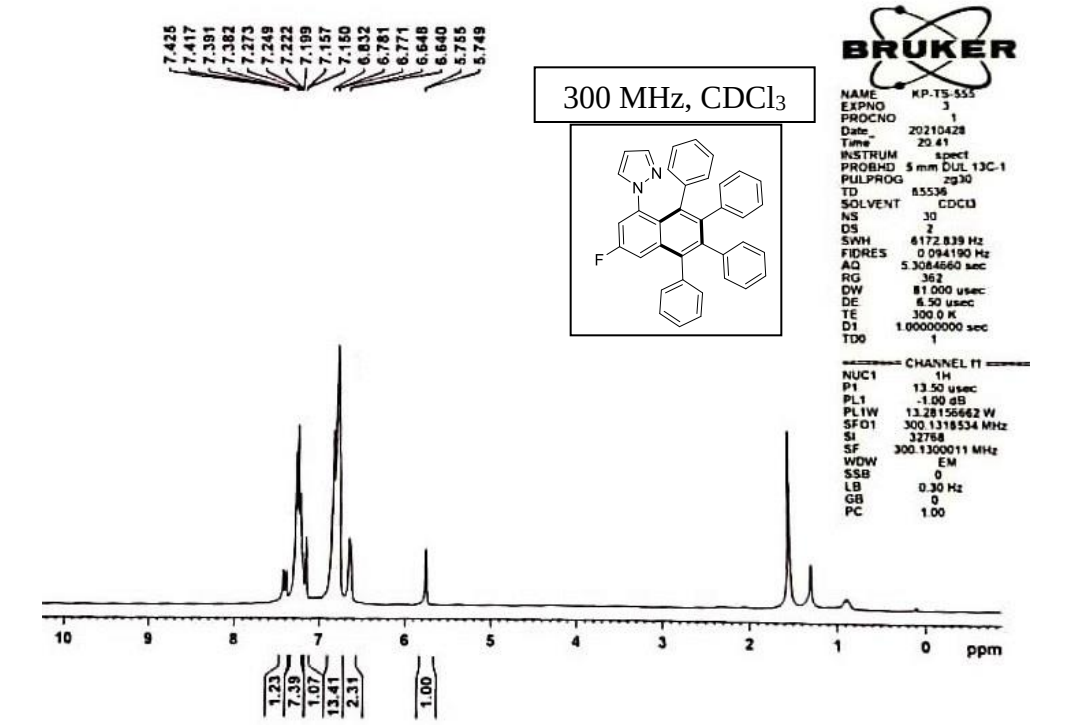
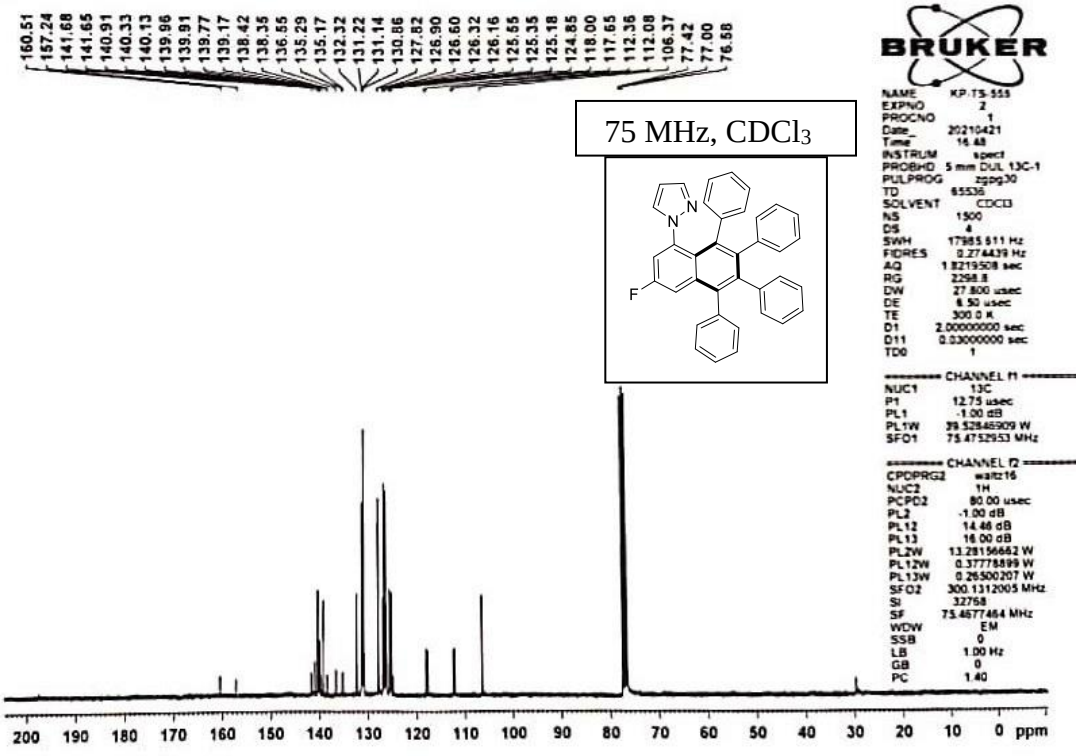
^{1}H and ^{13}C NMR spectra of compound **(3a)**



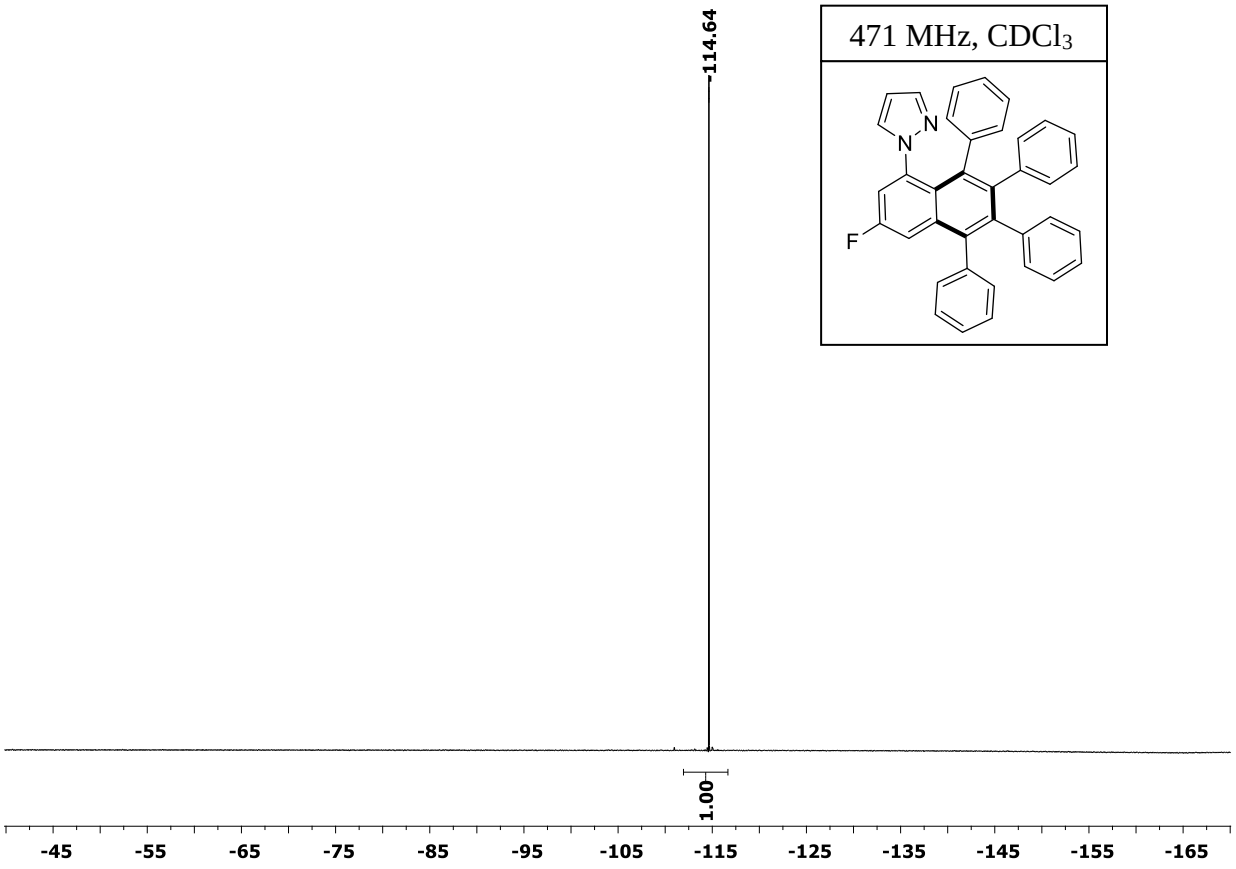


^{1}H and ^{13}C NMR spectra of compound **(3b)**

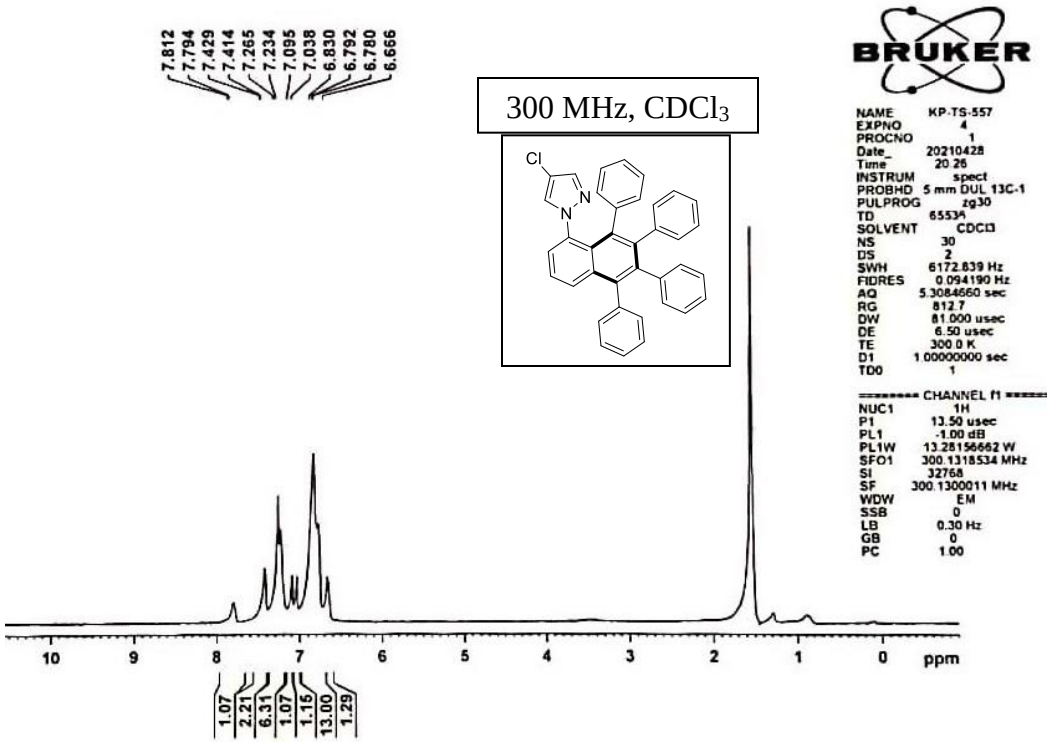


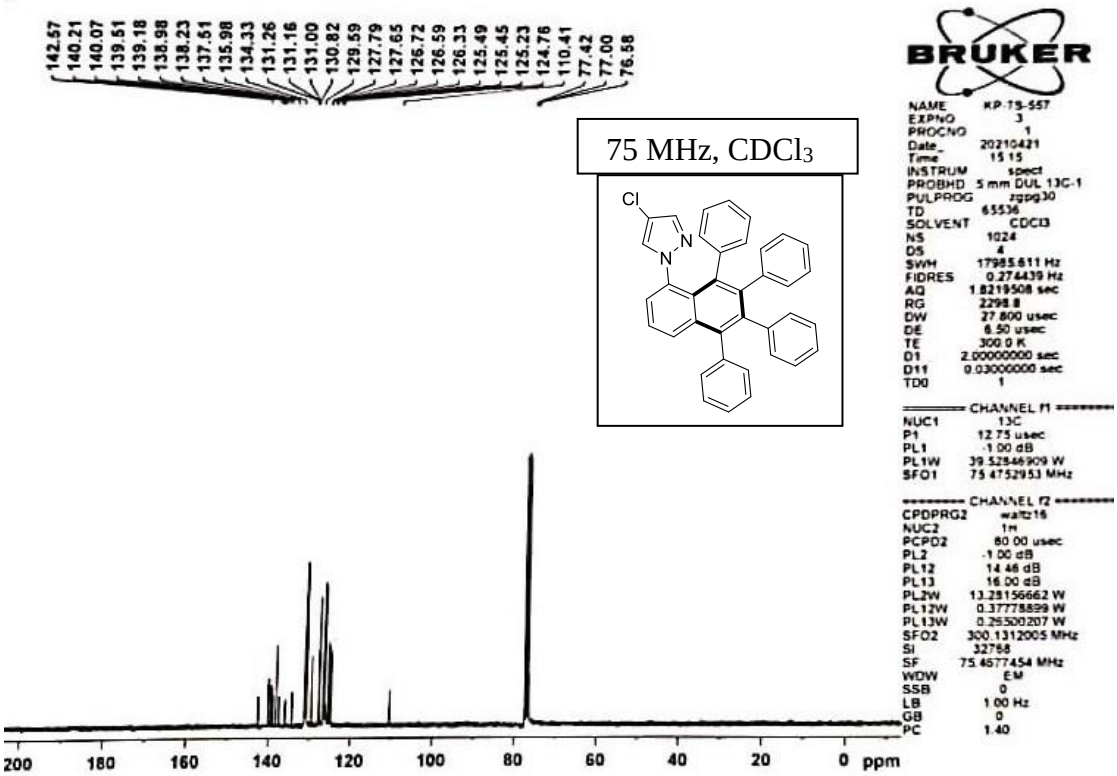


^{19}F NMR spectra of (3b)

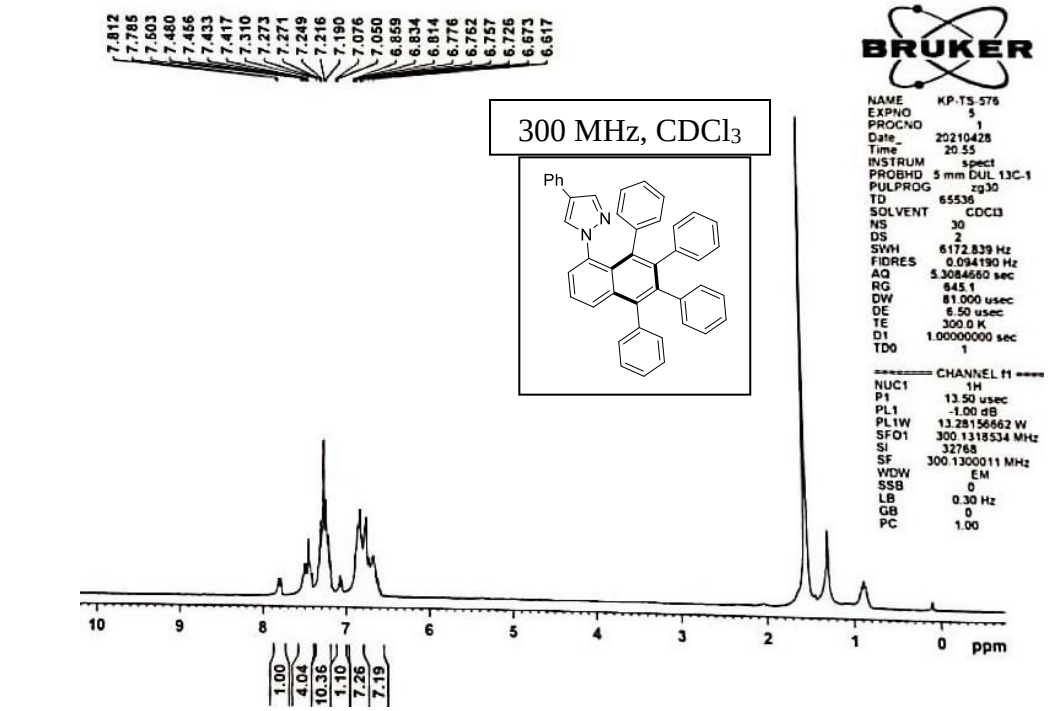


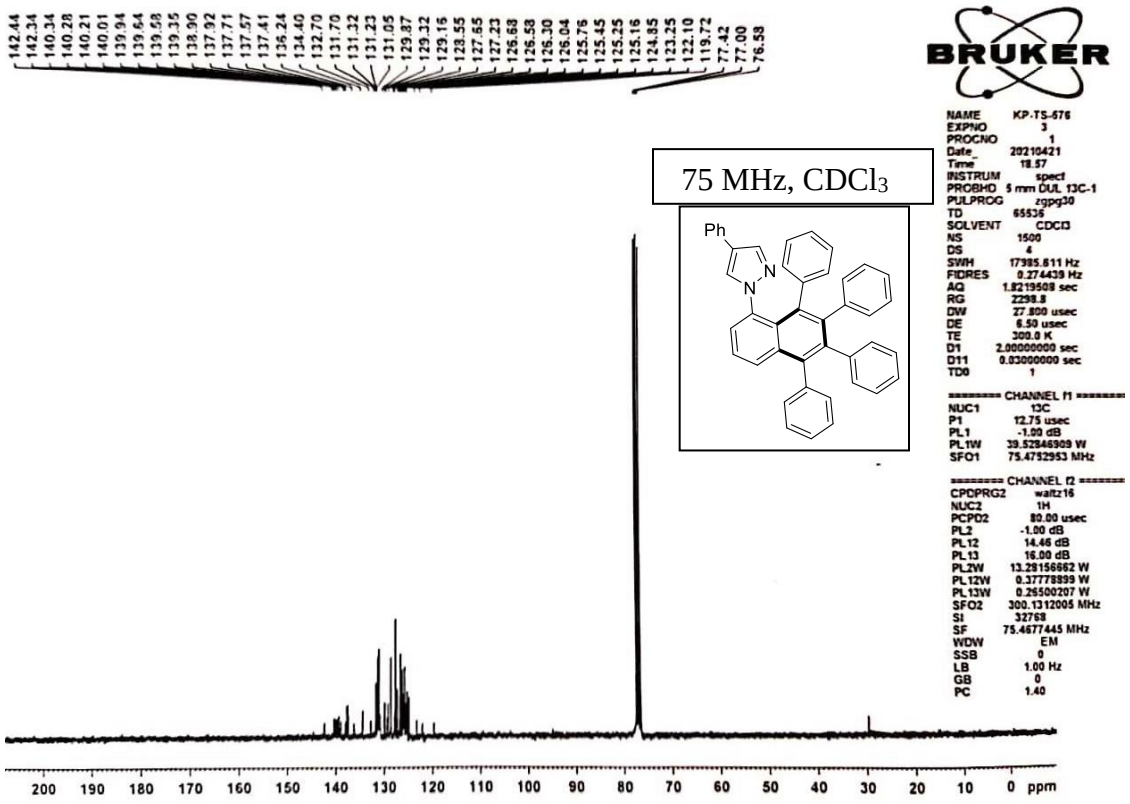
^{1}H and ^{13}C NMR spectra of compound **(3c)**



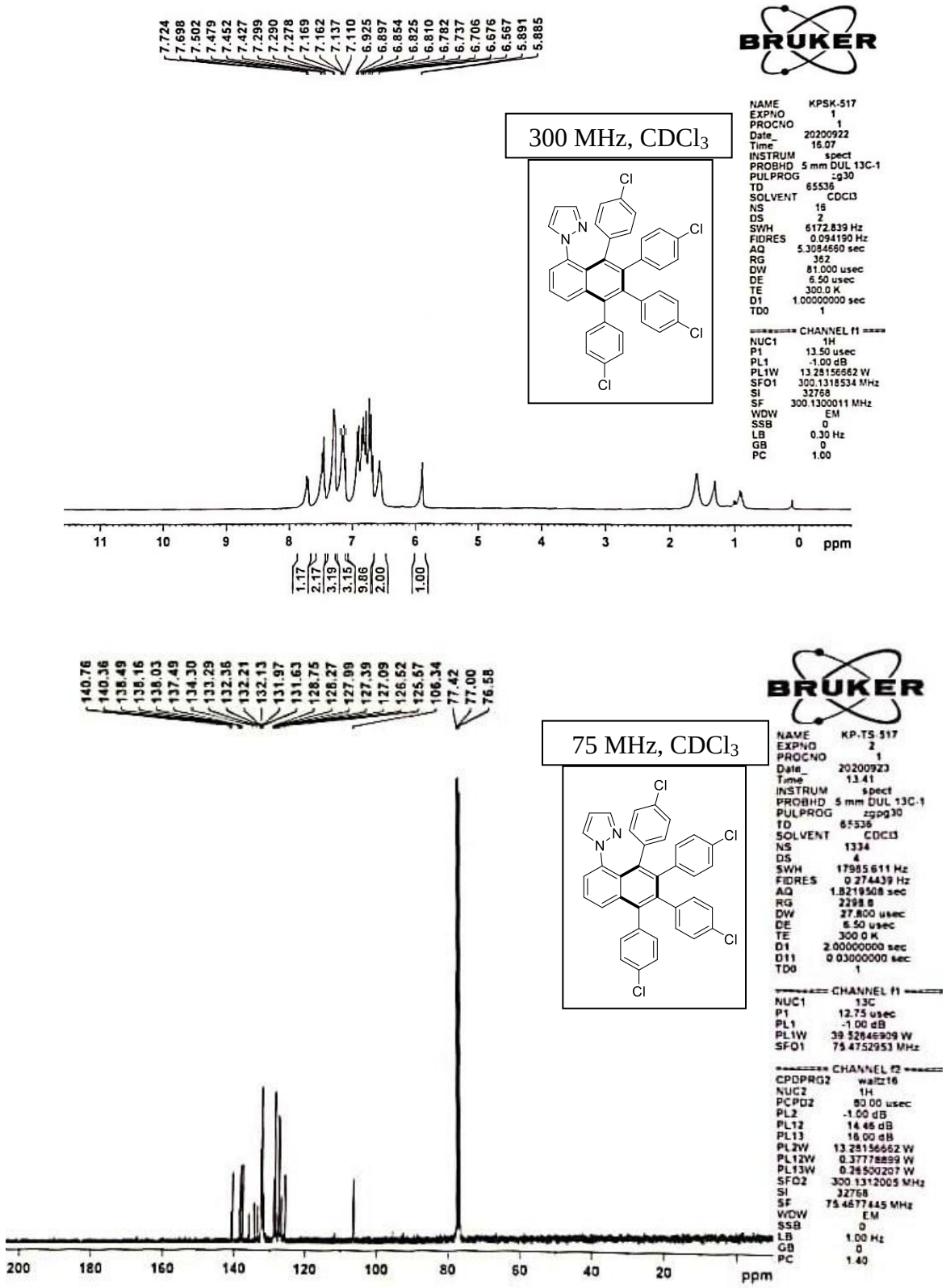


^{1}H and ^{13}C NMR spectra of compound **(3d)**

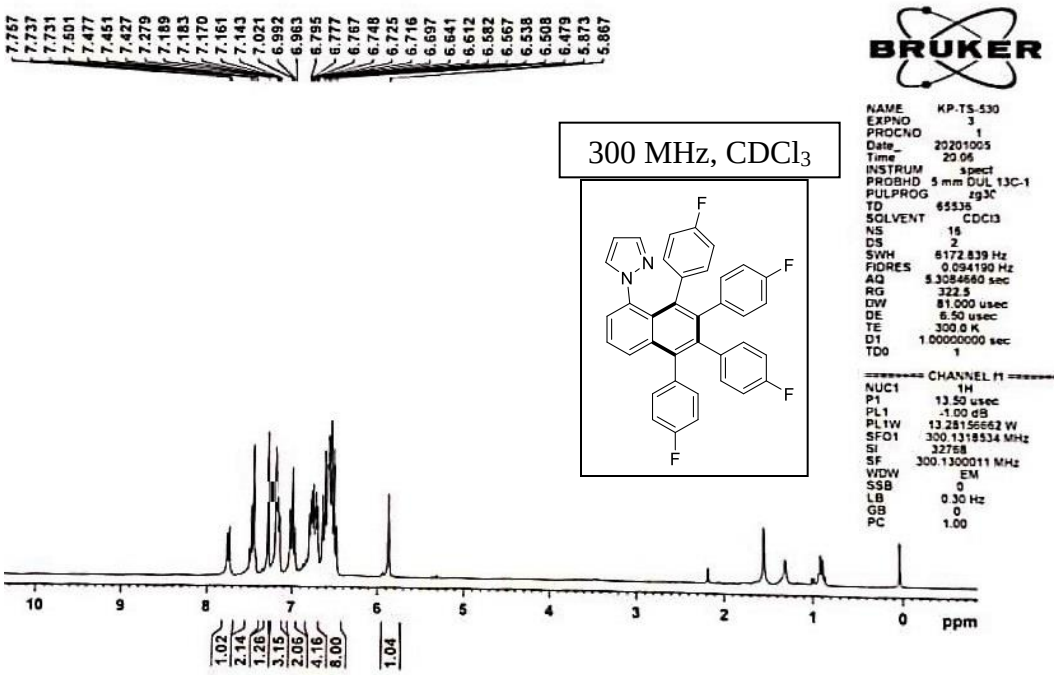


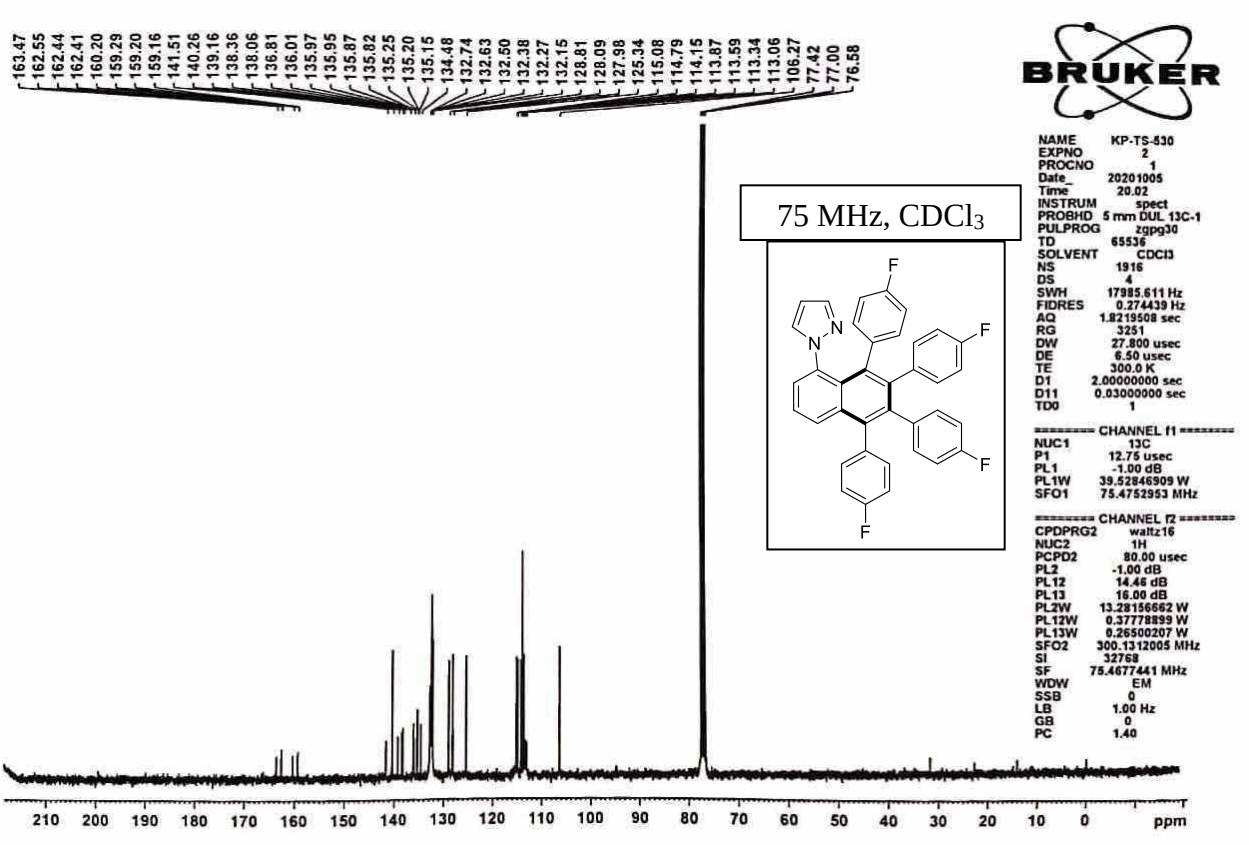


^{1}H and ^{13}C NMR spectra of compound **(3e)**

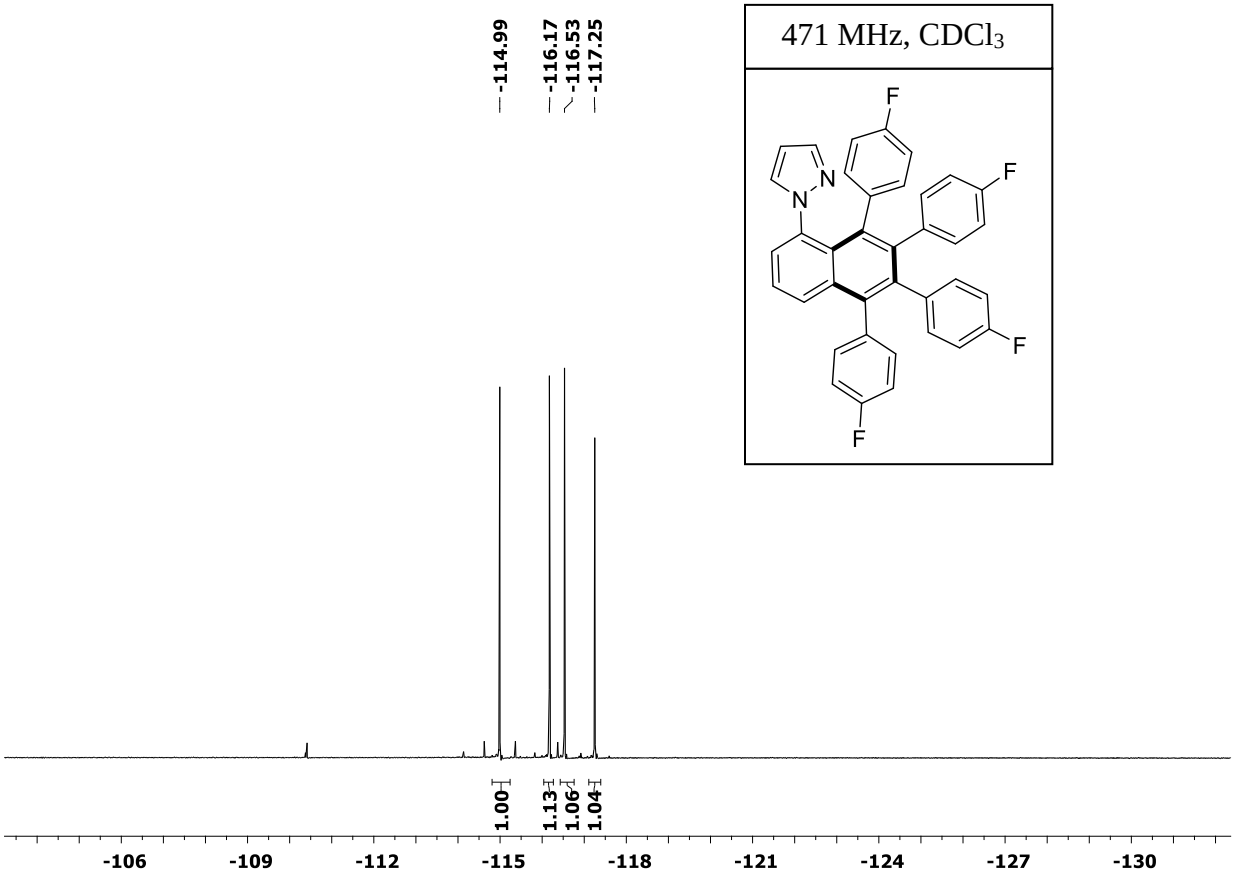


^{1}H and ^{13}C NMR spectra of compound **(3f)**

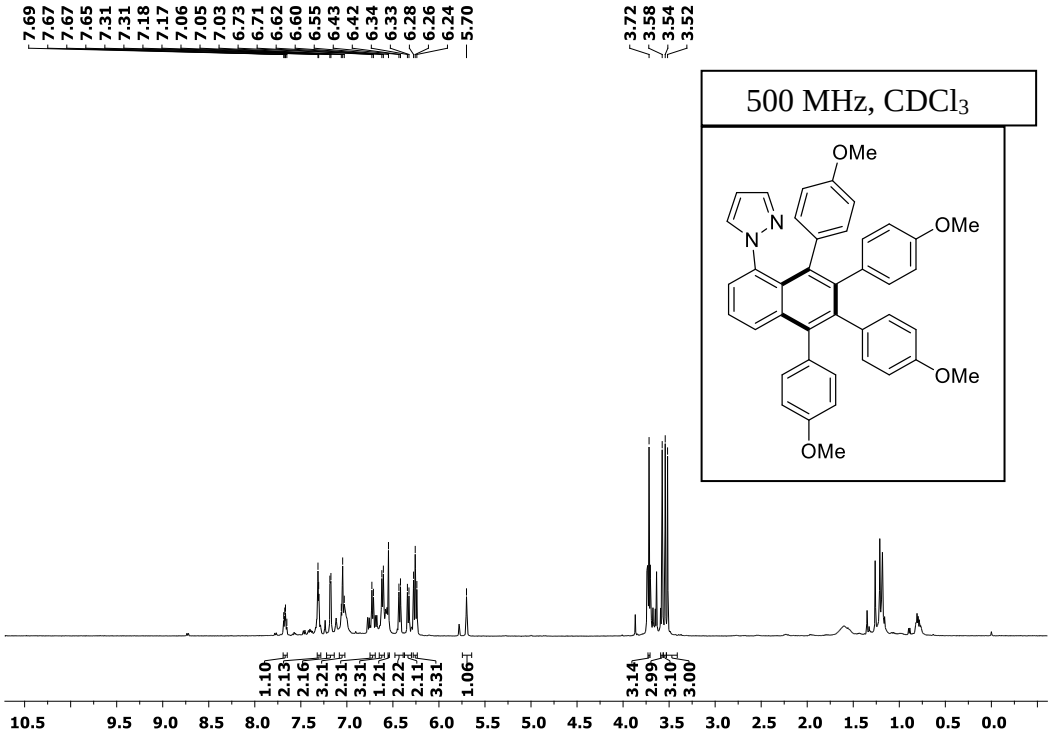


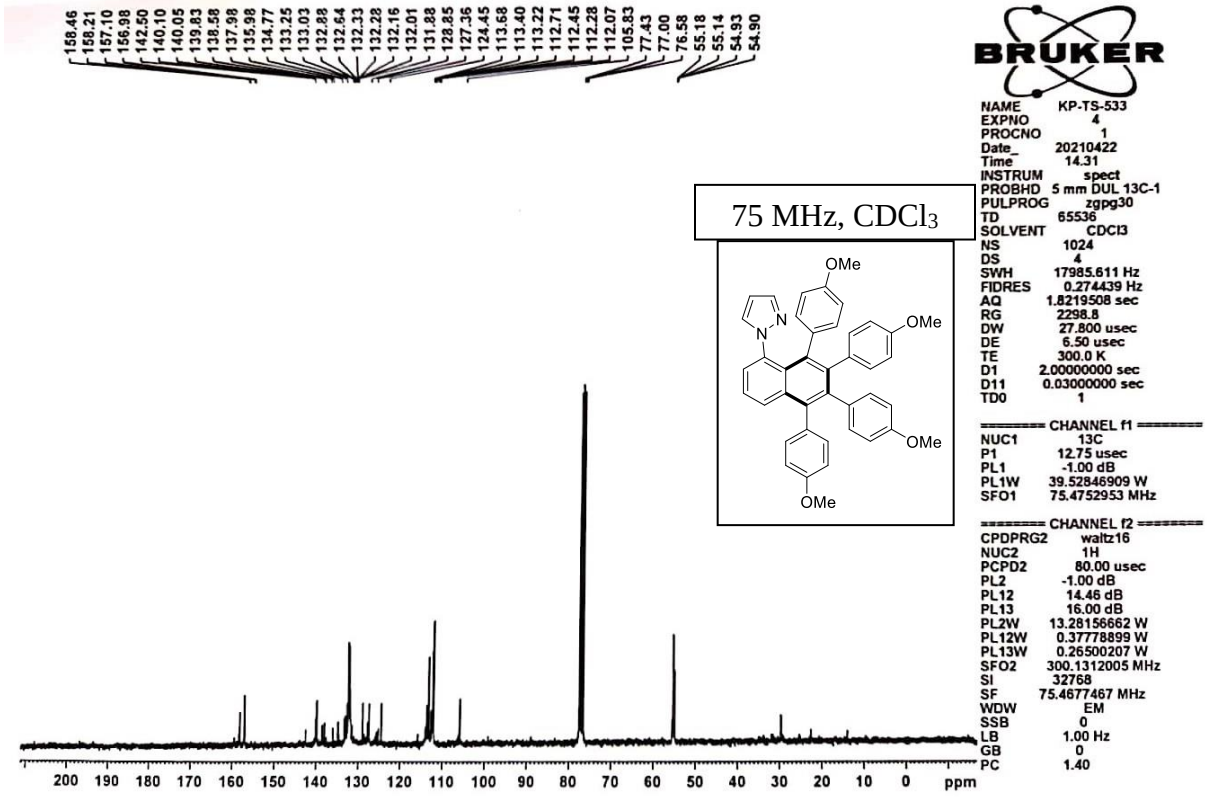


^{19}F NMR spectra of (3f)



^{1}H and ^{13}C NMR spectra of compound **(3g)**





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DE	6.50 usec
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PL1W	39.52848909 W
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PCPD2	80.00 usec
PL2	-1.00 dB
PL12	14.46 dB
PL13	16.00 dB
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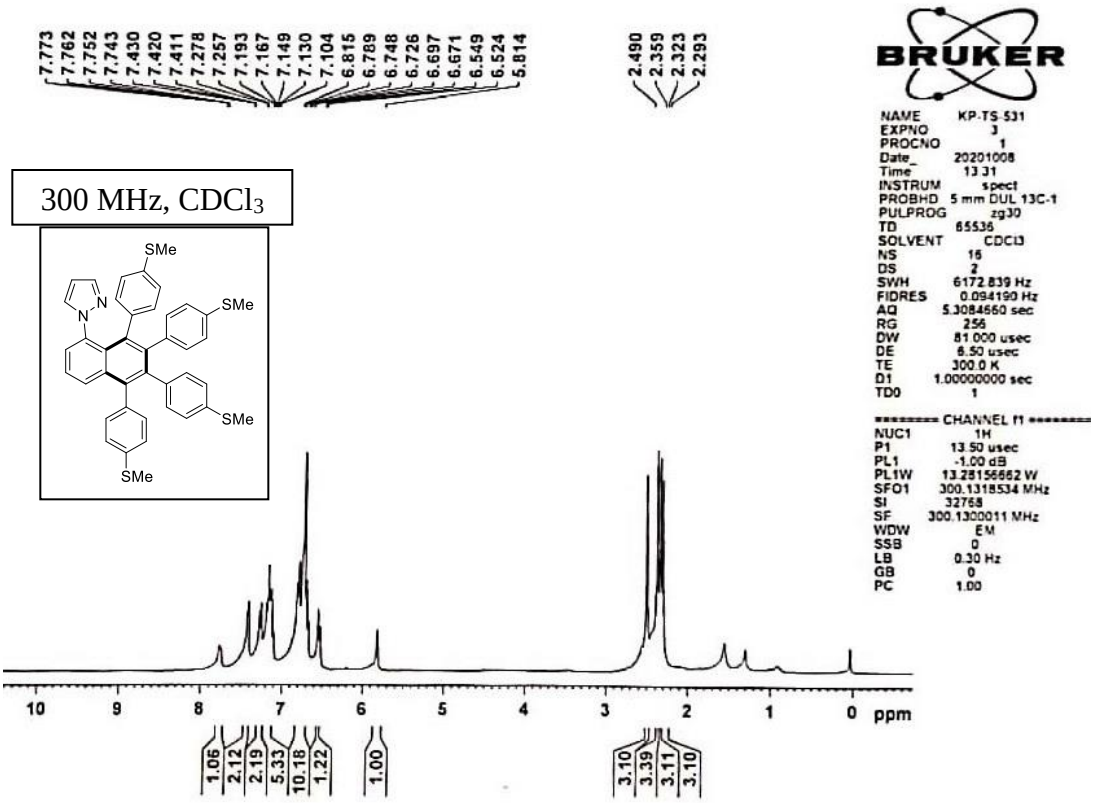
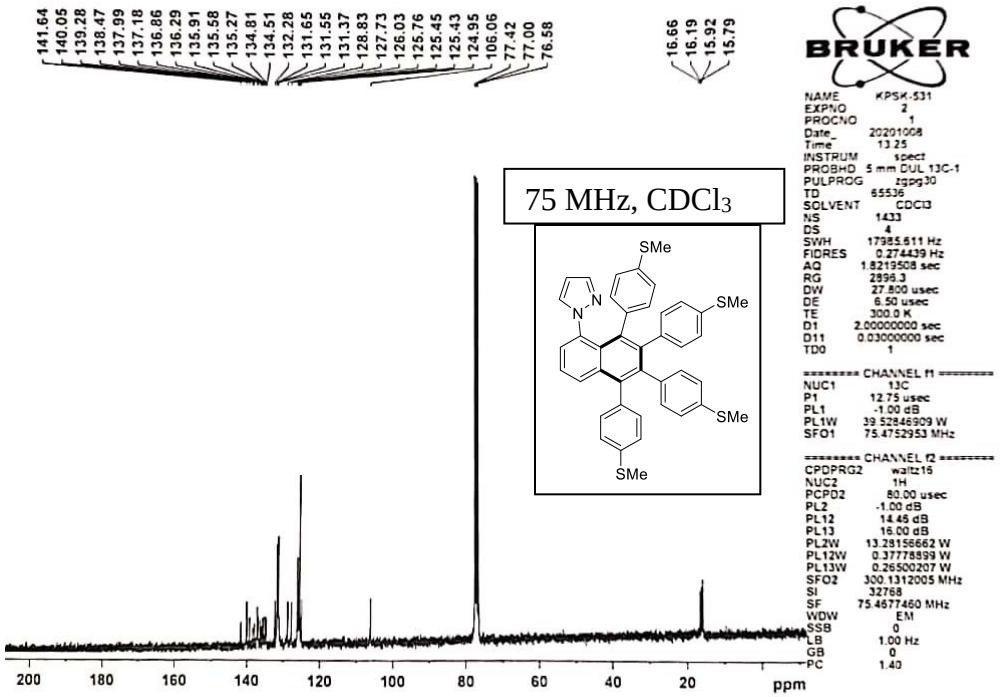
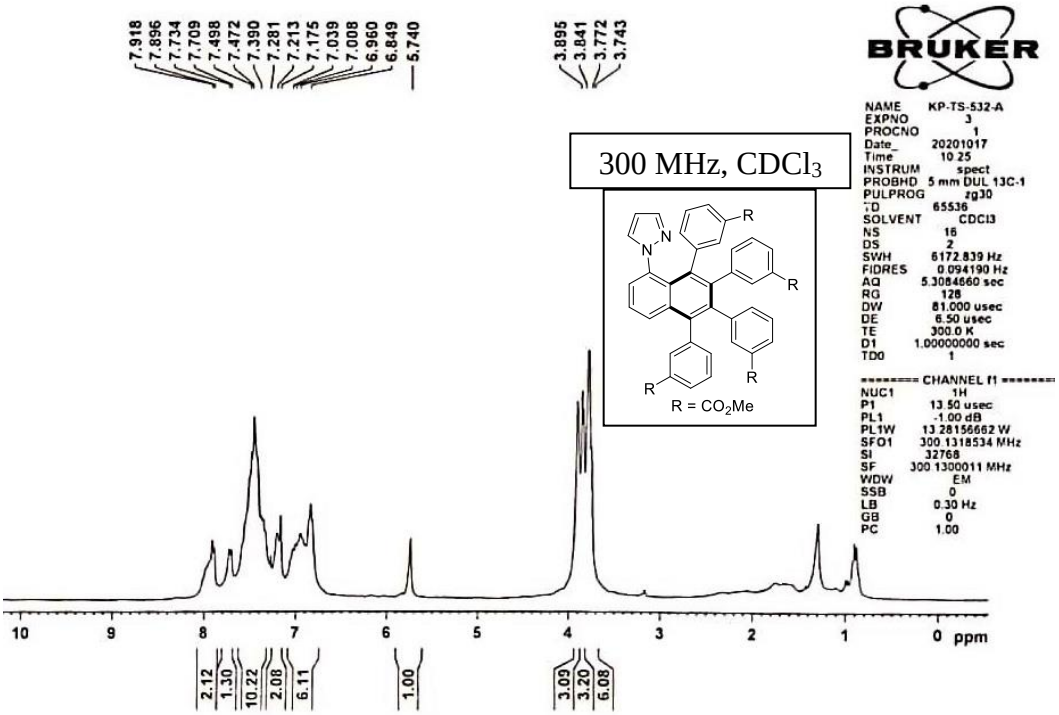
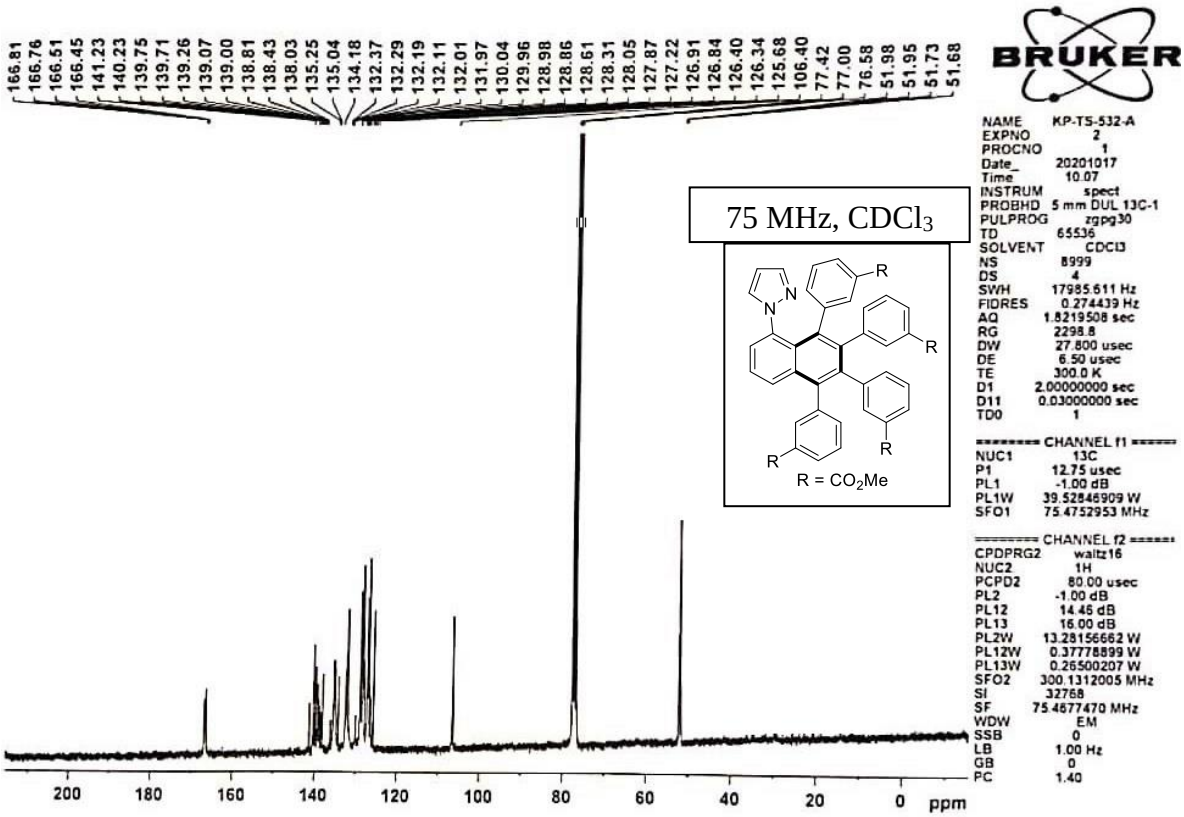
^{1}H and ^{13}C NMR spectra of compound **(3h)**



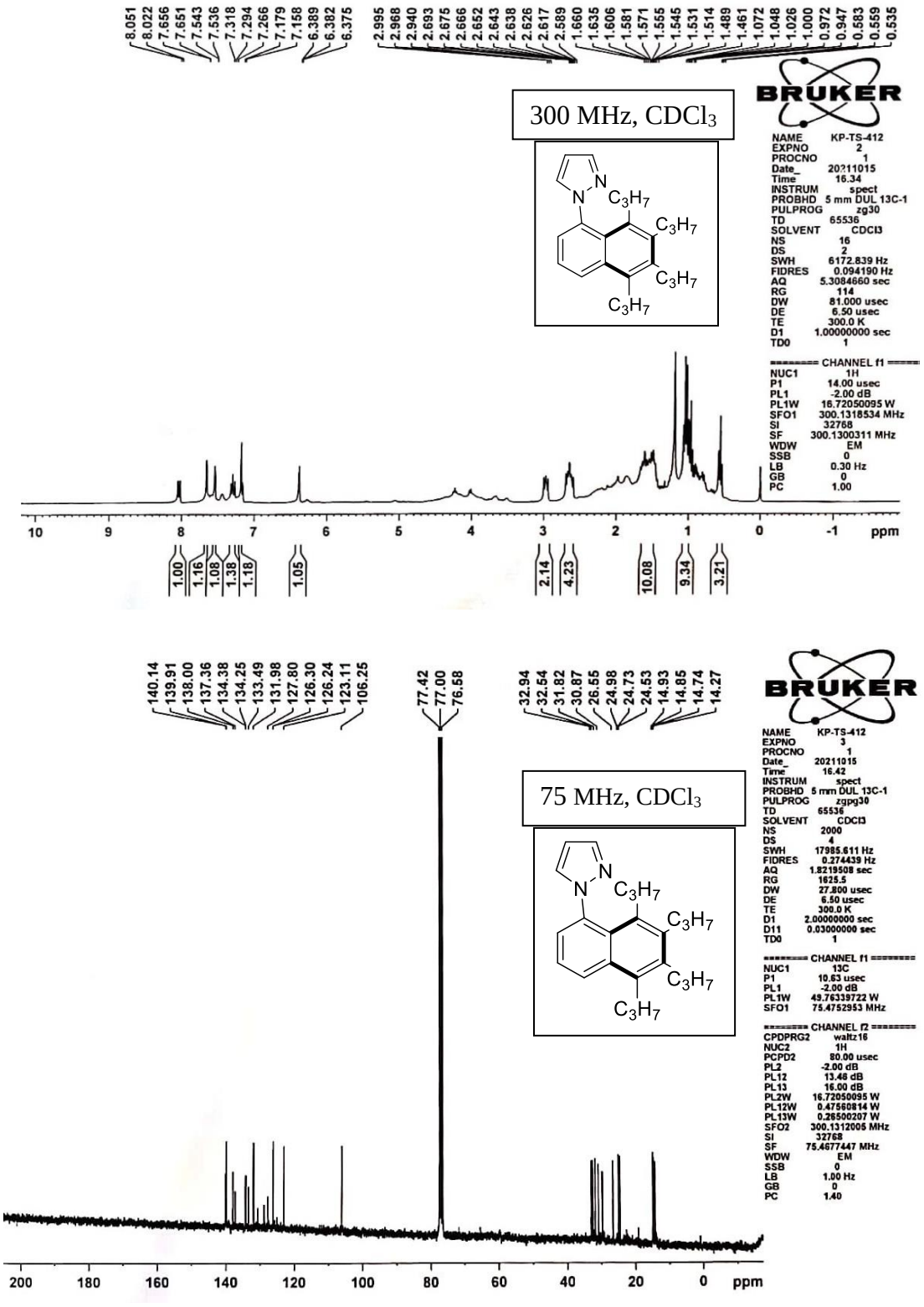


^{1}H and ^{13}C NMR spectra of compound **(3i)**

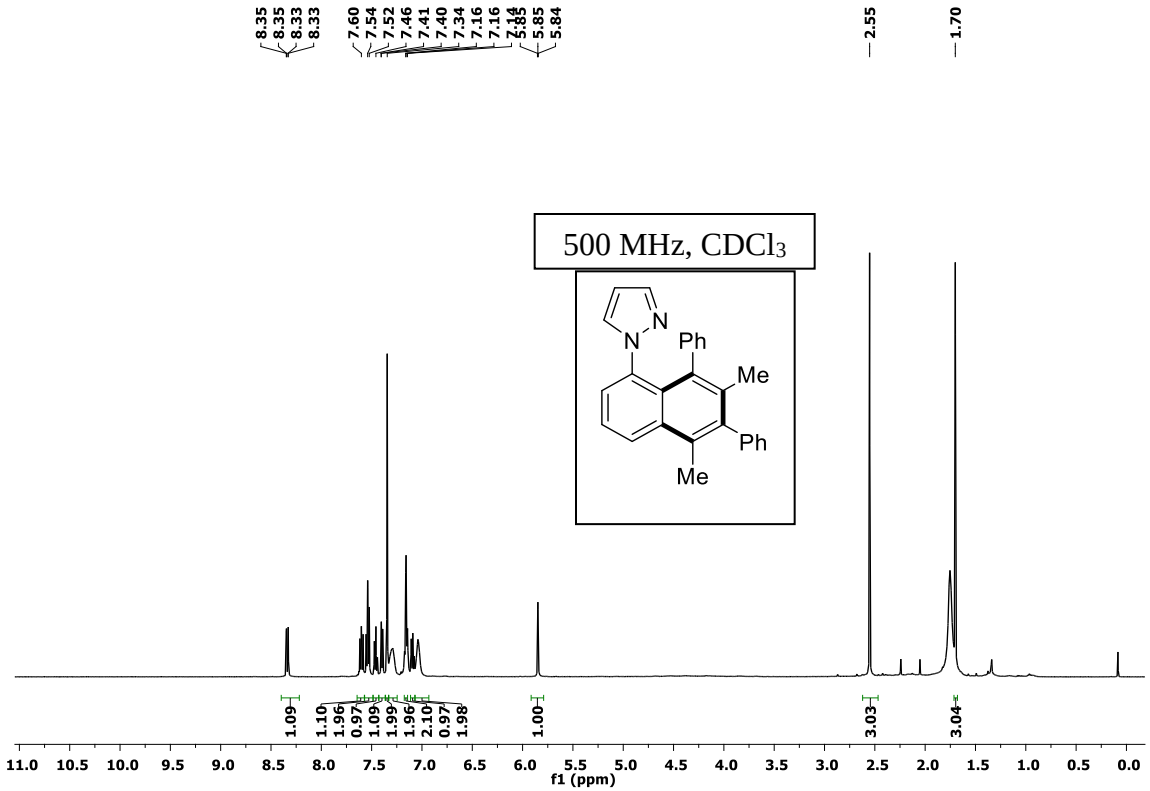


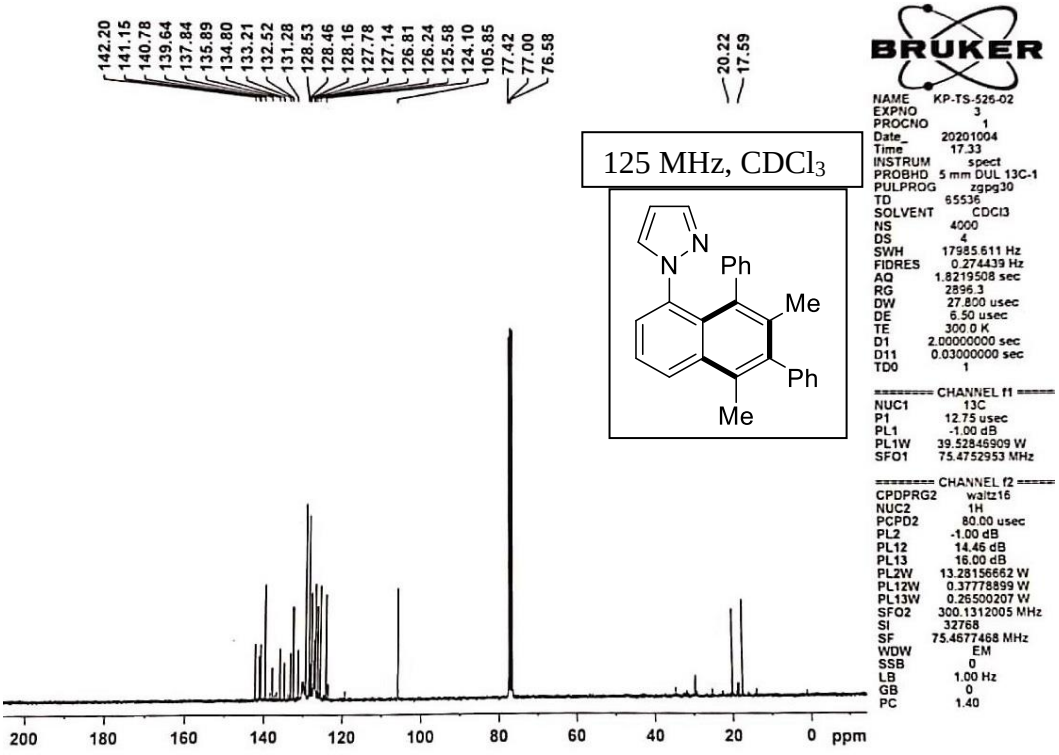


^{1}H and ^{13}C NMR spectra of compound **(3j)**



^{1}H and ^{13}C NMR spectra of compound **(3k)**





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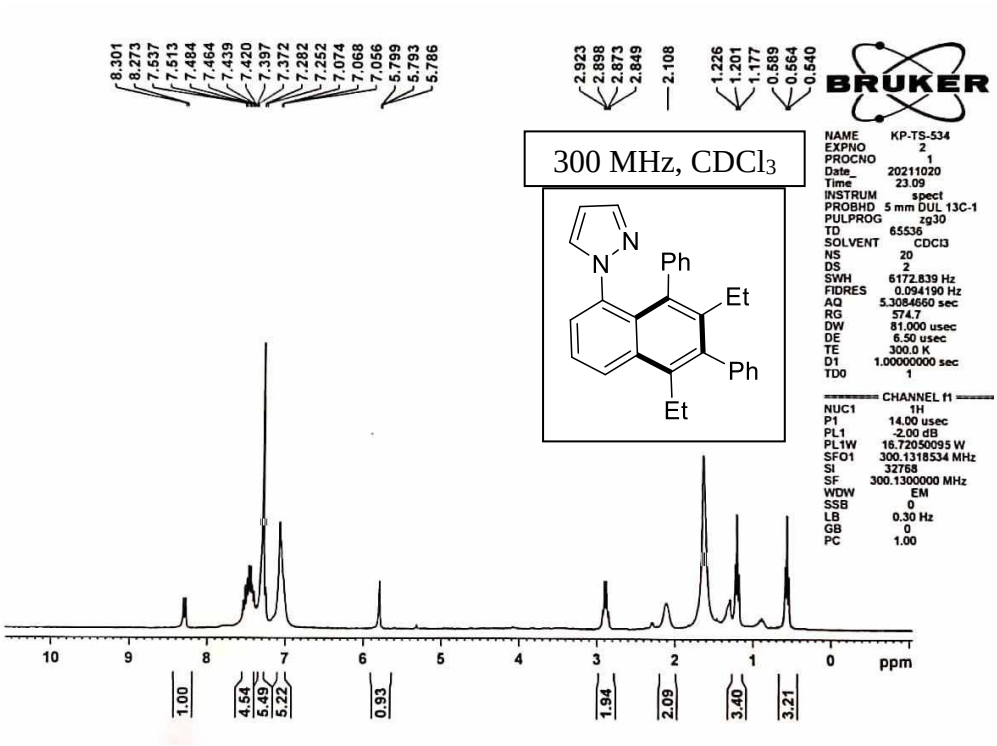
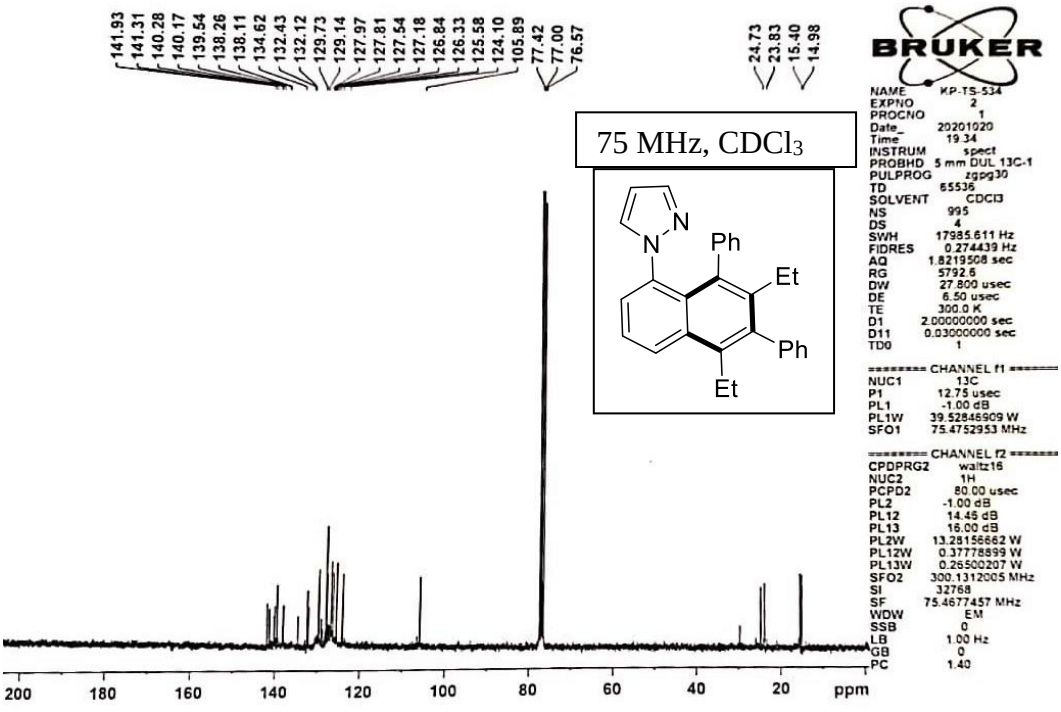
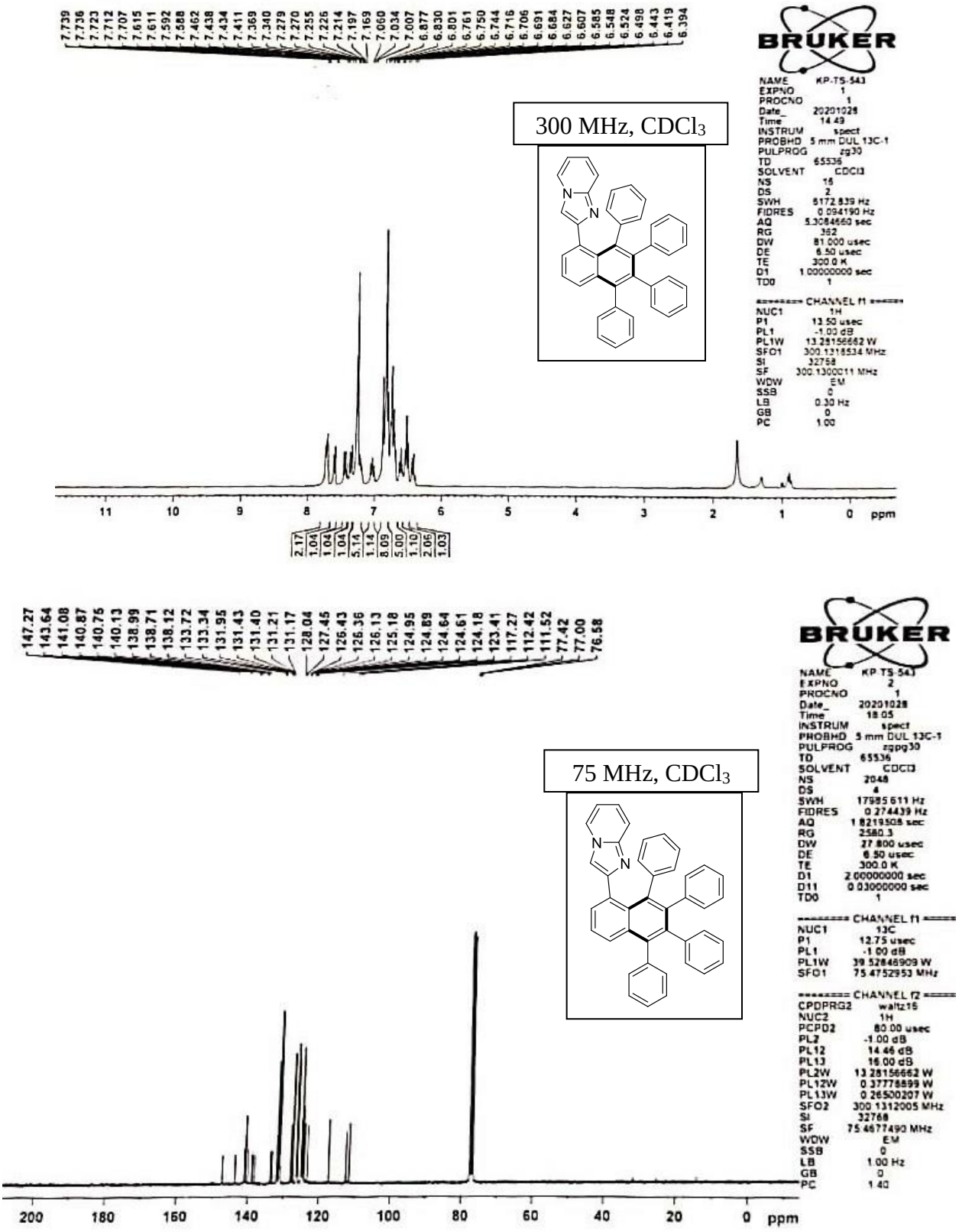
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2896.3
DW	27.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ======	
NUC1	13C
P1	12.75 usec
PL1	-1.00 dB
PL1W	39.52846909 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	14.46 dB
PL13	16.00 dB
PL2W	13.28156662 W
PL12W	0.37778899 W
PL13W	0.26500207 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677468 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

^{1}H and ^{13}C NMR spectra of compound **(3l)**

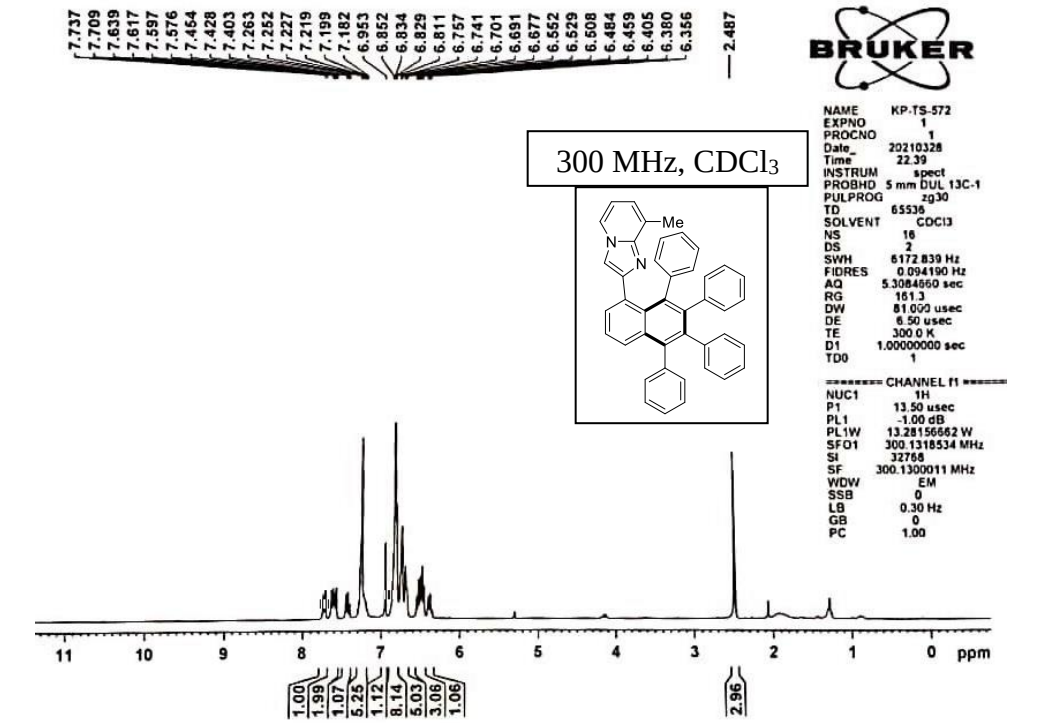


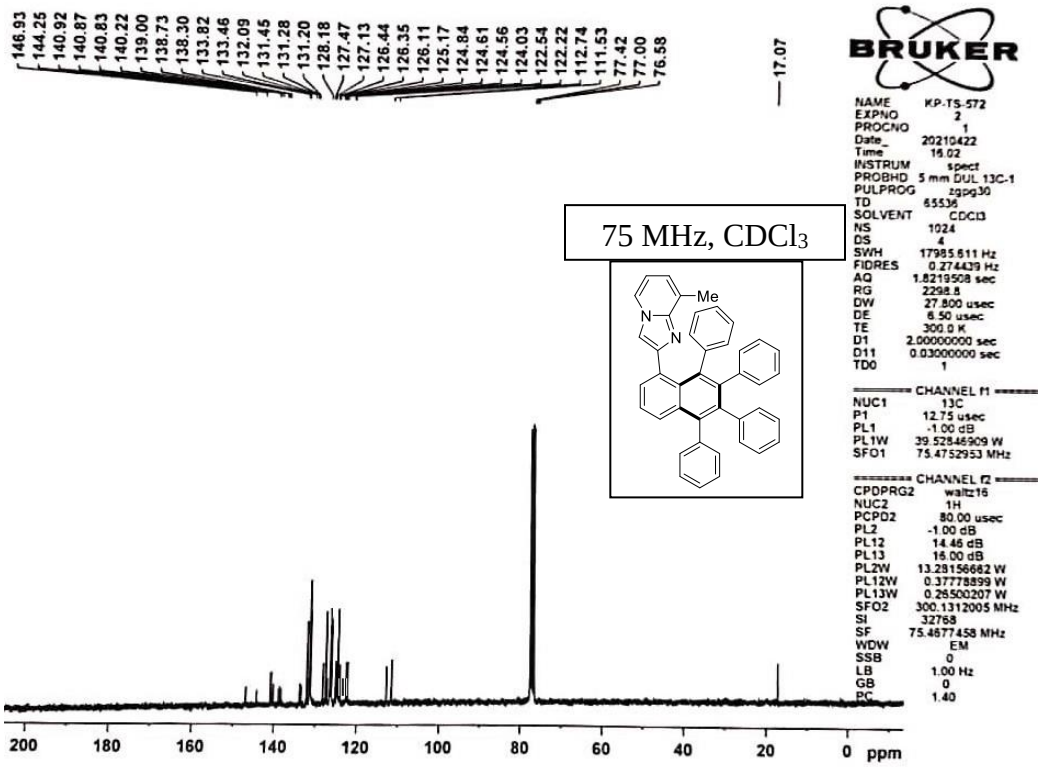


^{1}H and ^{13}C NMR spectra of compound **(5a)**

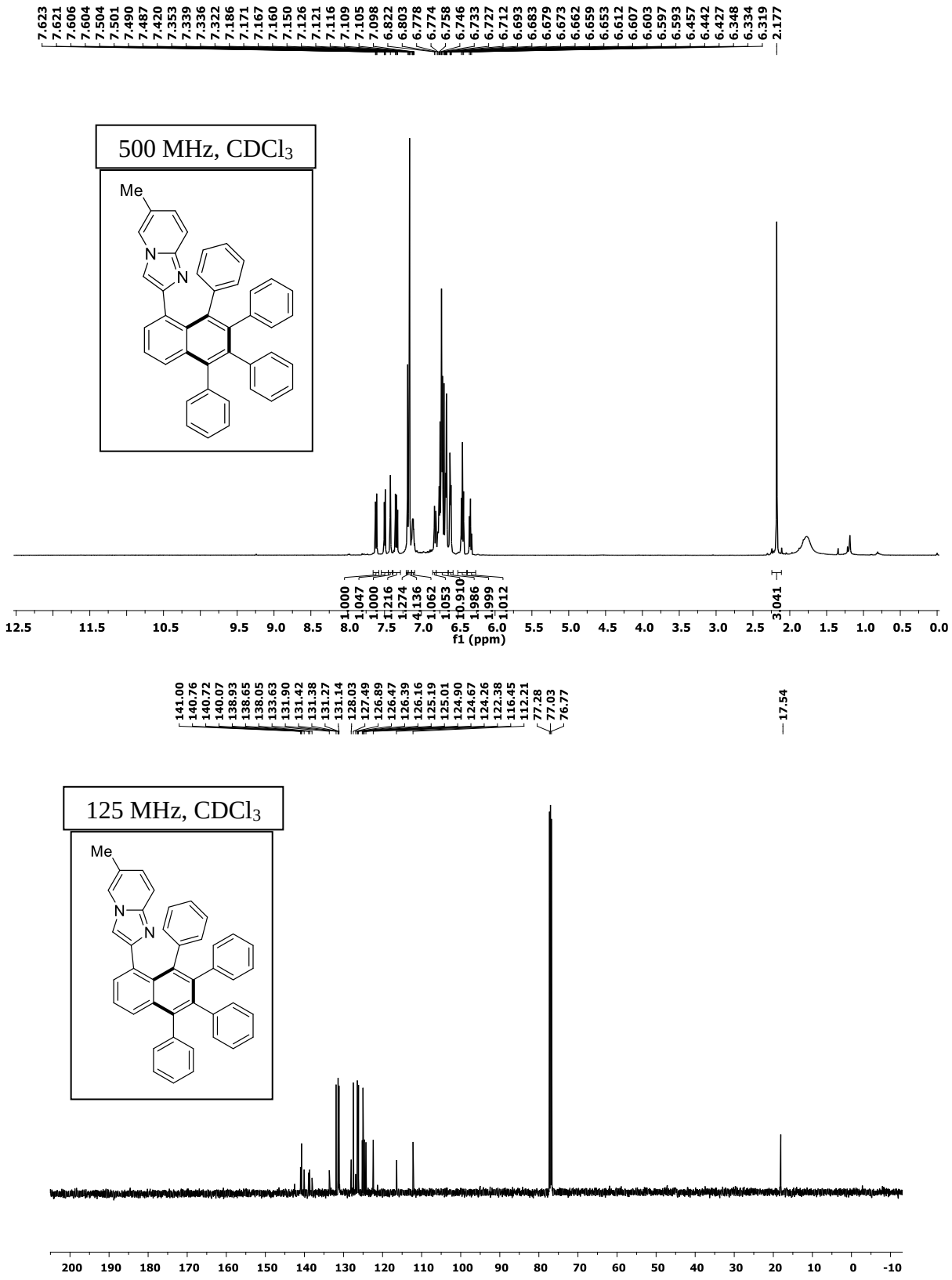


^{1}H and ^{13}C NMR spectra of compound **(5b)**

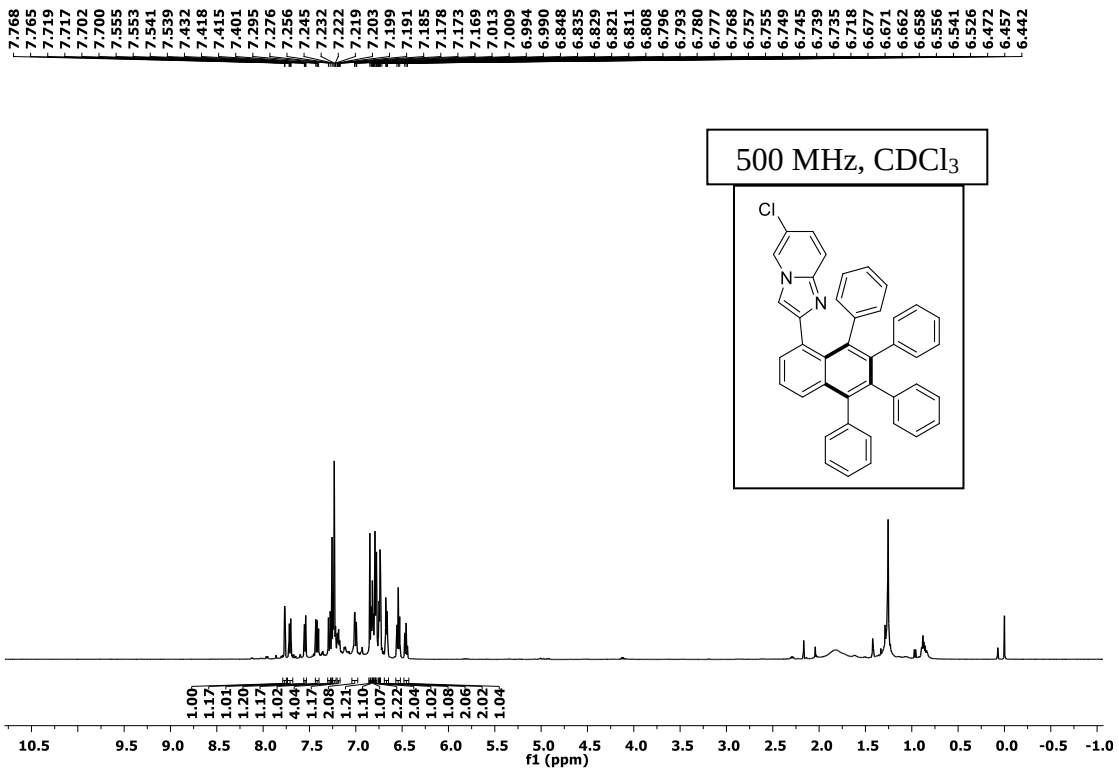


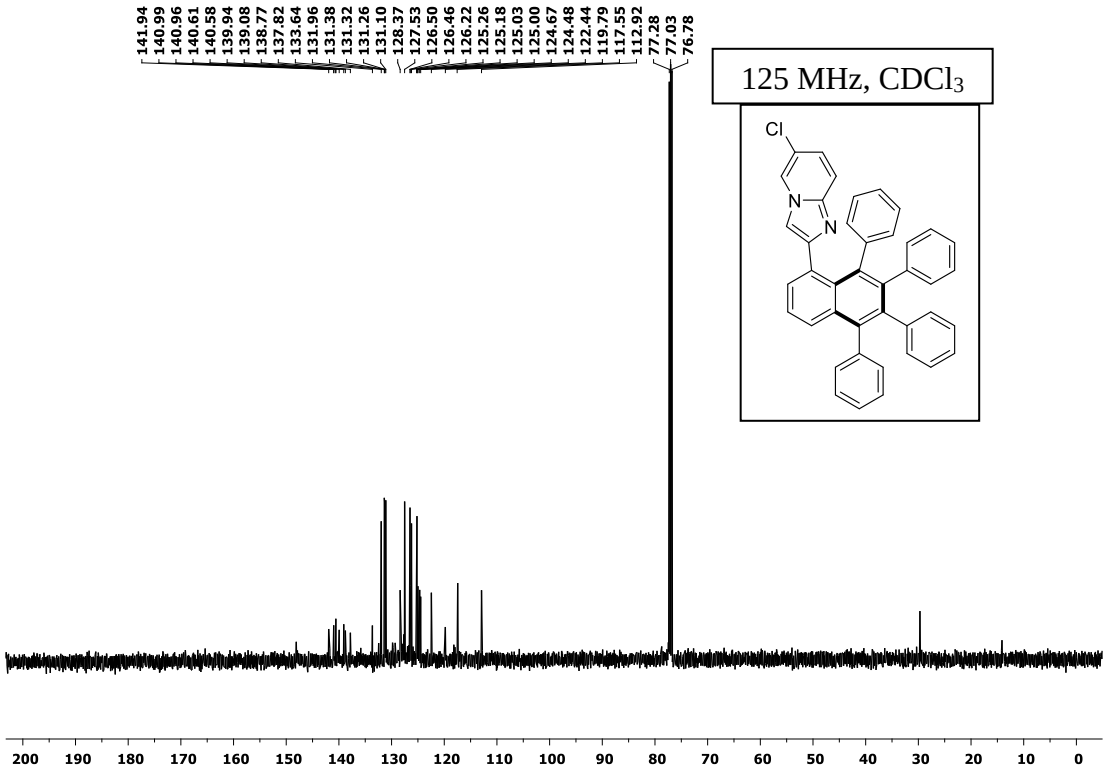


^{1}H and ^{13}C NMR spectra of compound **(5c)**

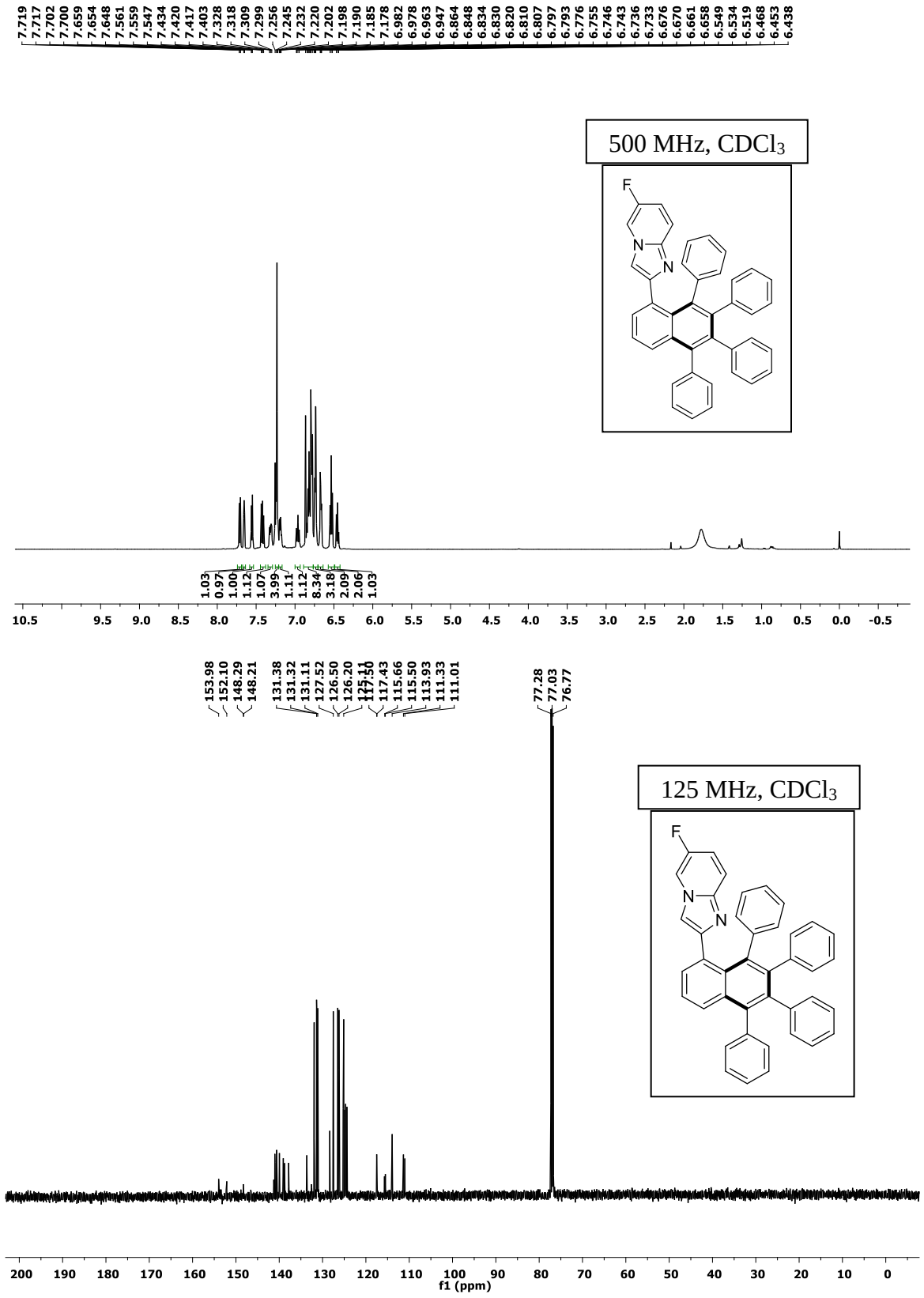


^{1}H and ^{13}C NMR spectra of compound **(5d)**

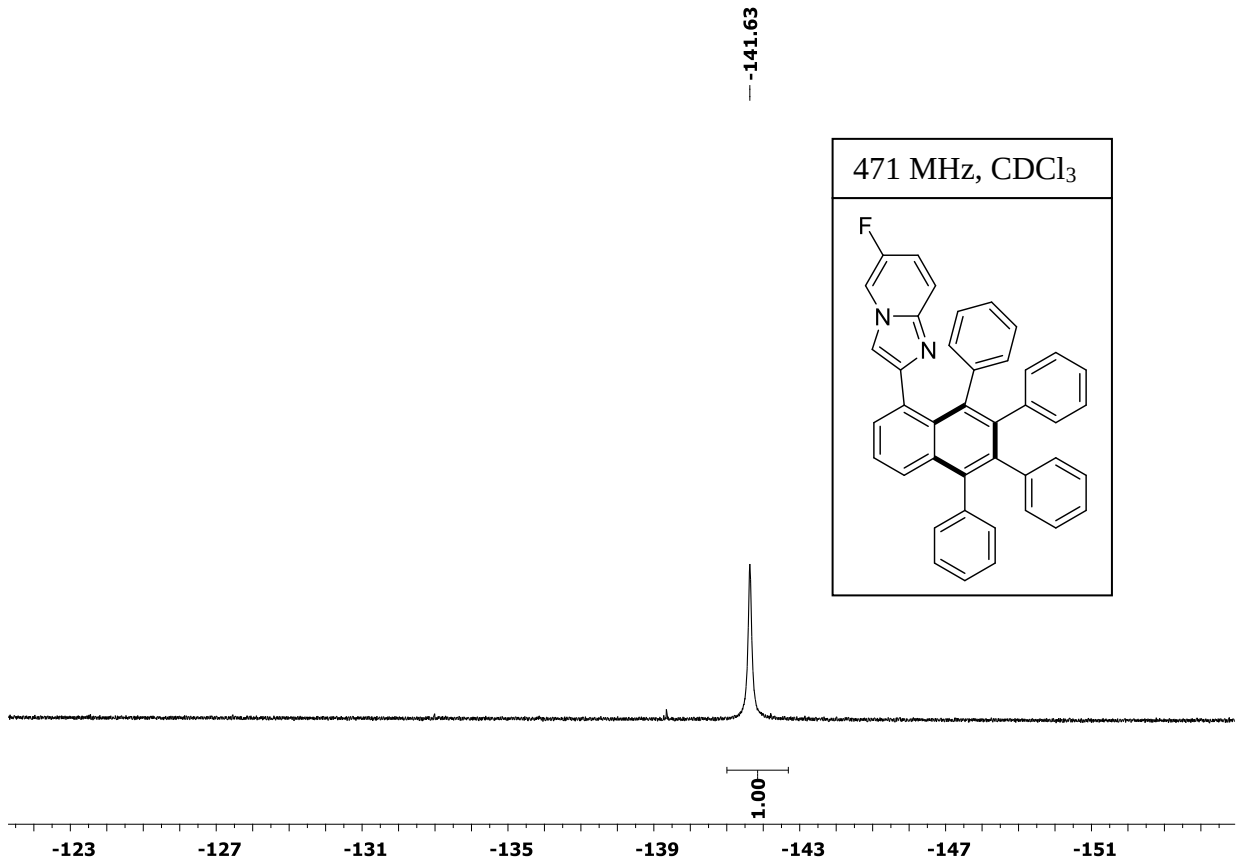




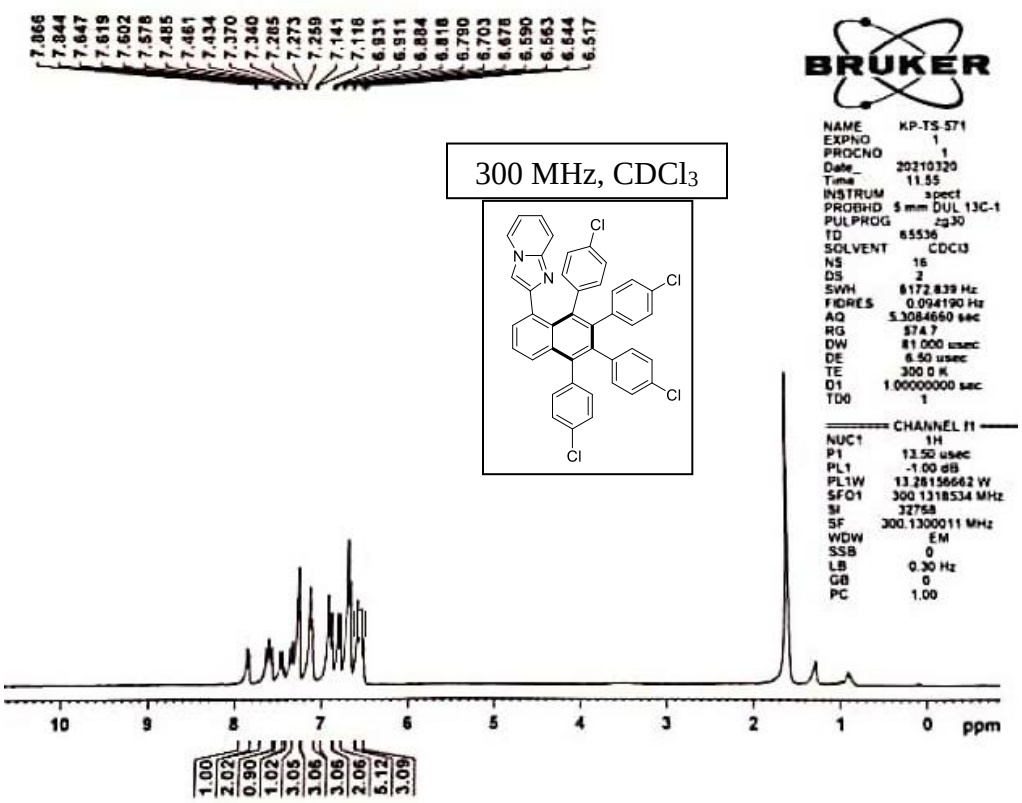
^{1}H and ^{13}C NMR spectra of compound **(5e)**

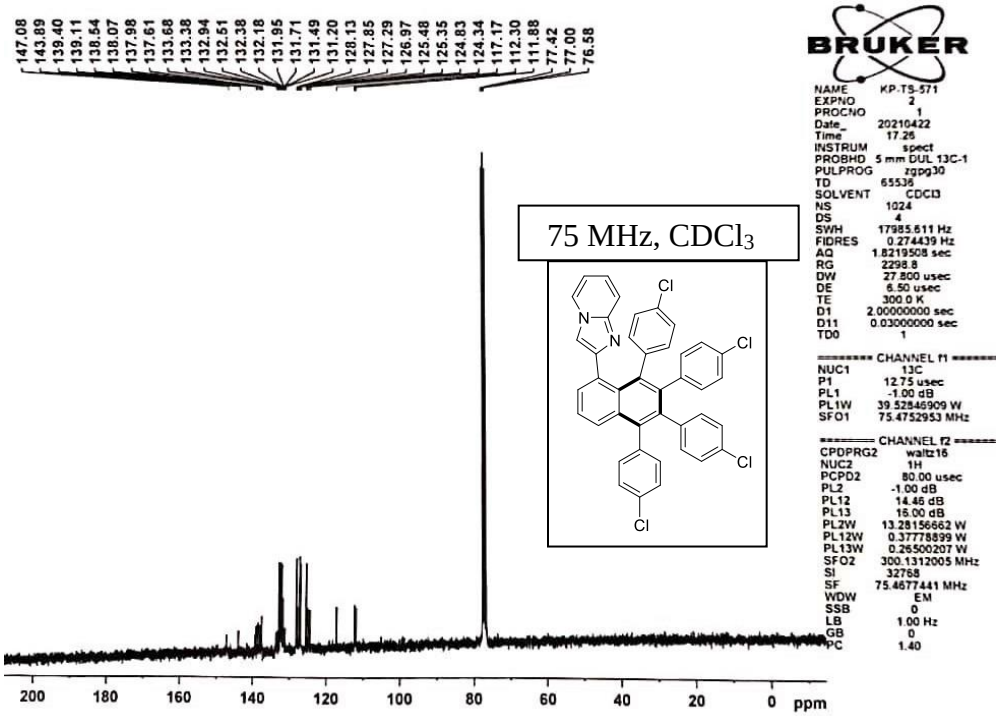


^{19}F NMR spectra of (5e)

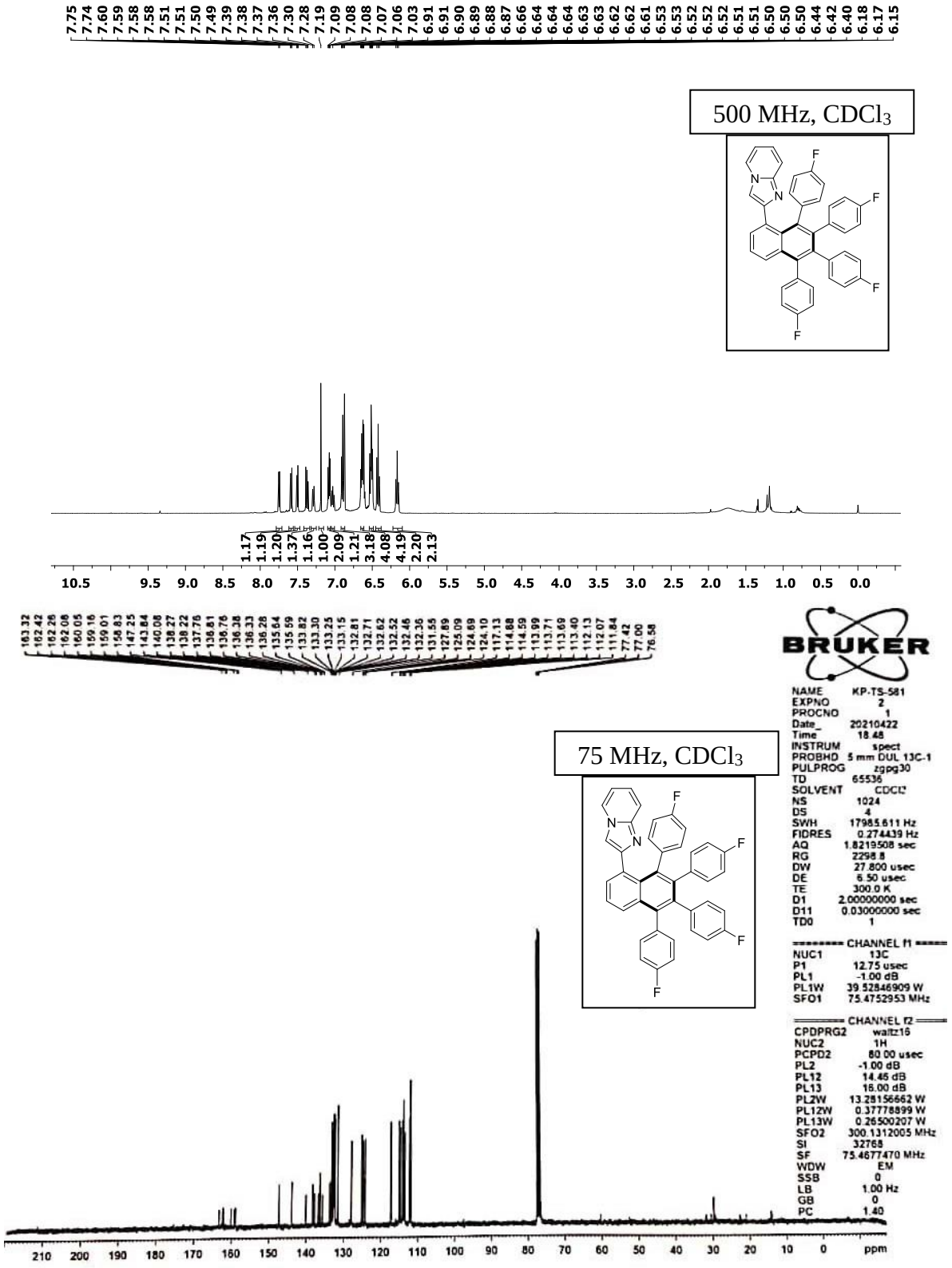


^{1}H and ^{13}C NMR spectra of compound **(5g)**

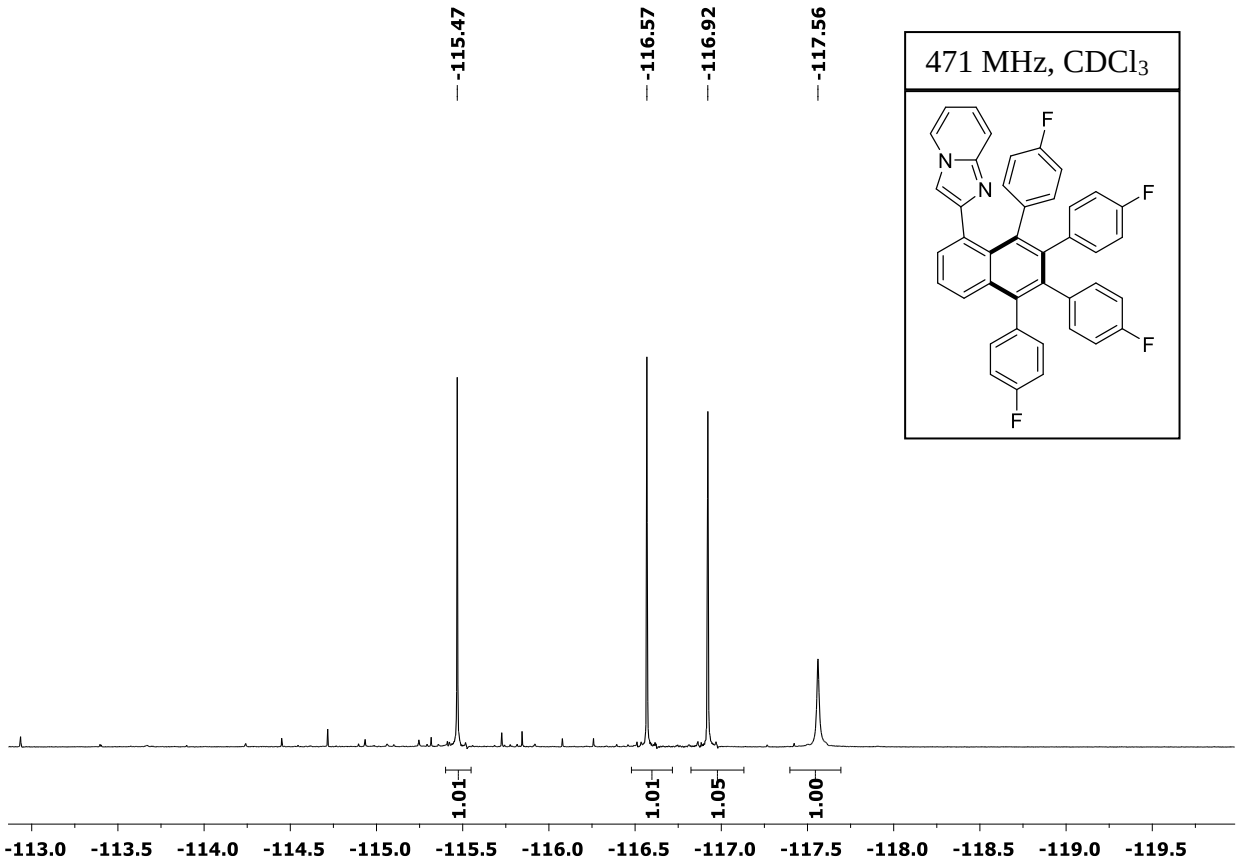




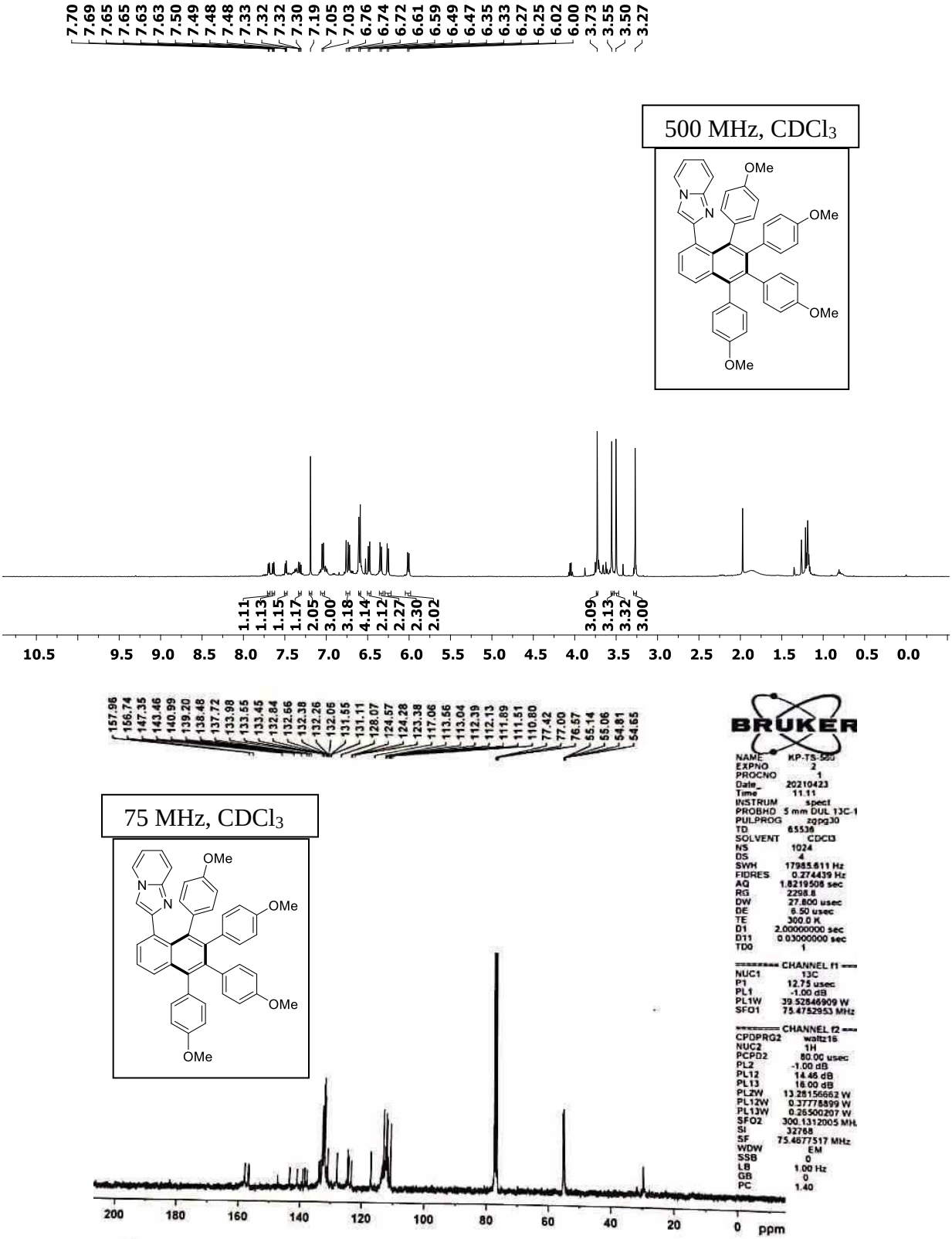
^{1}H and ^{13}C NMR spectra of compound **(5h)**



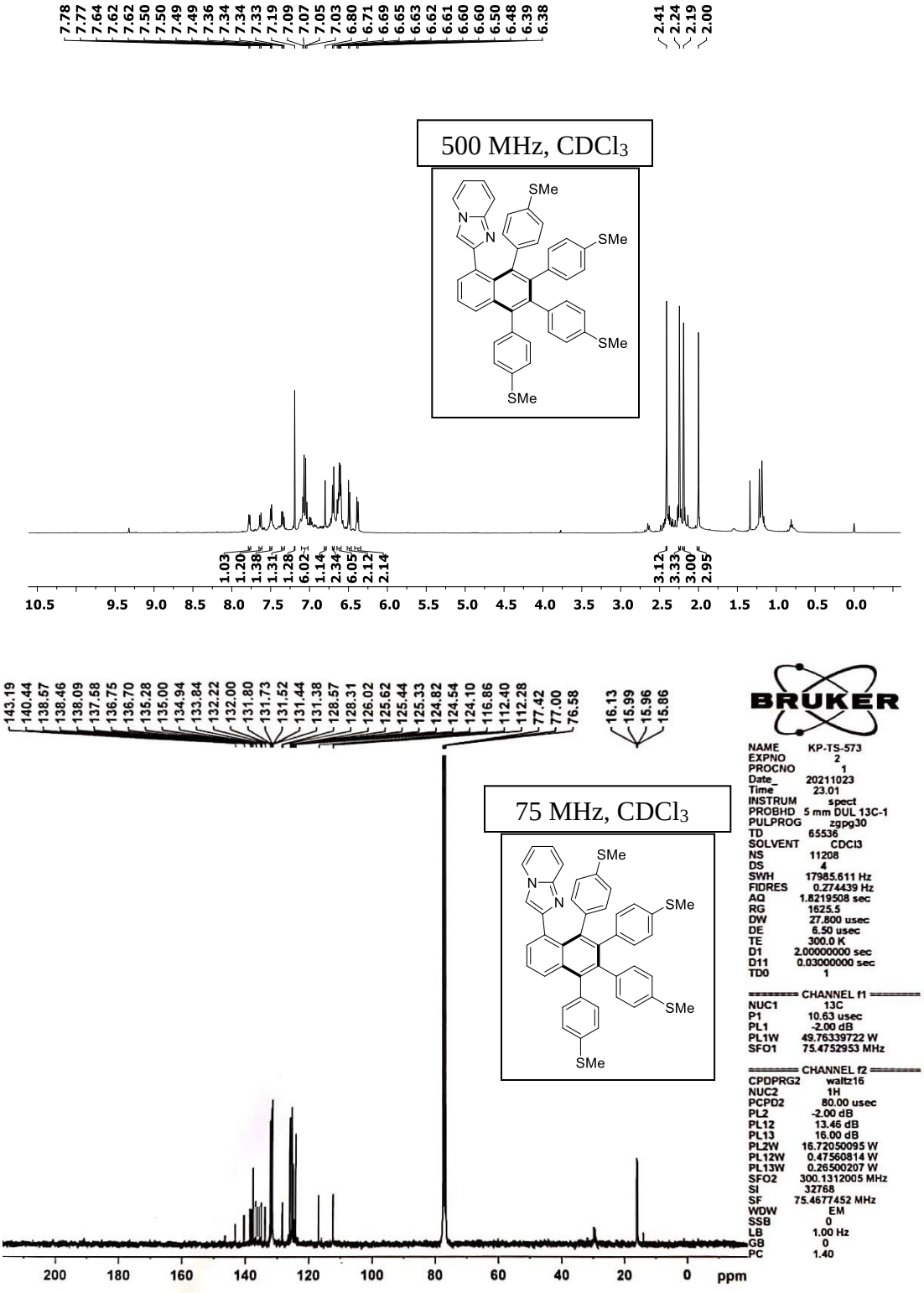
^{19}F NMR spectra of (5h)



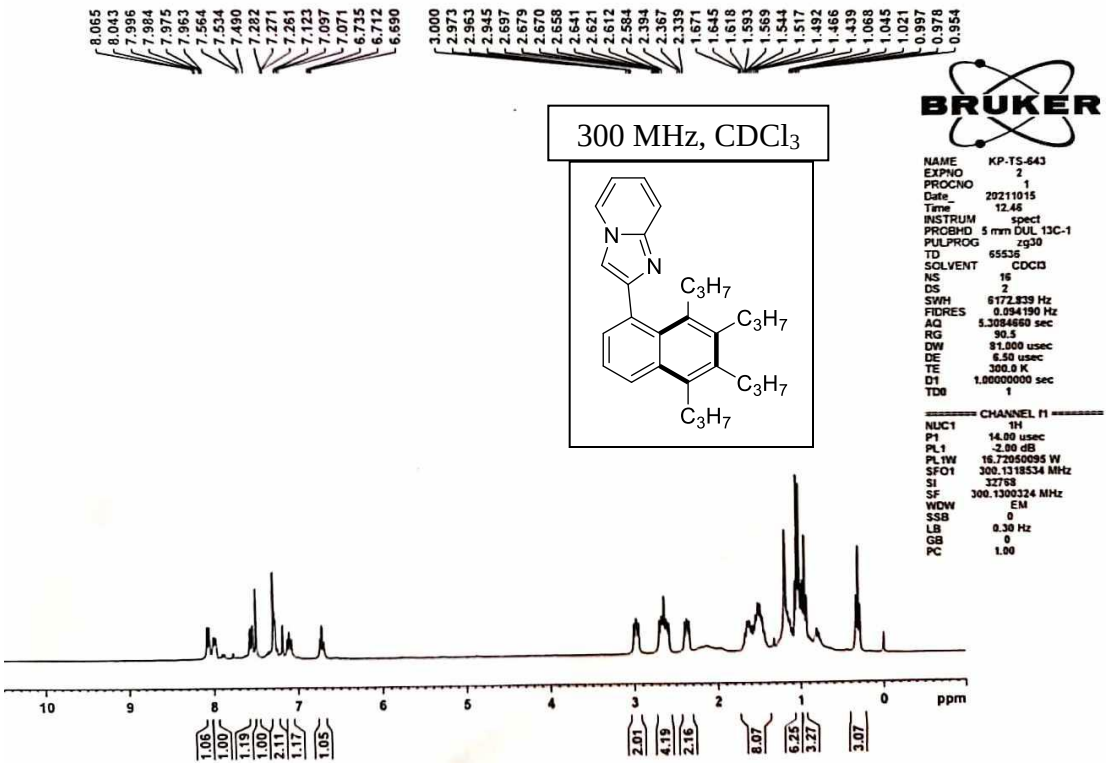
^{1}H and ^{13}C NMR spectra of compound **(5i)**

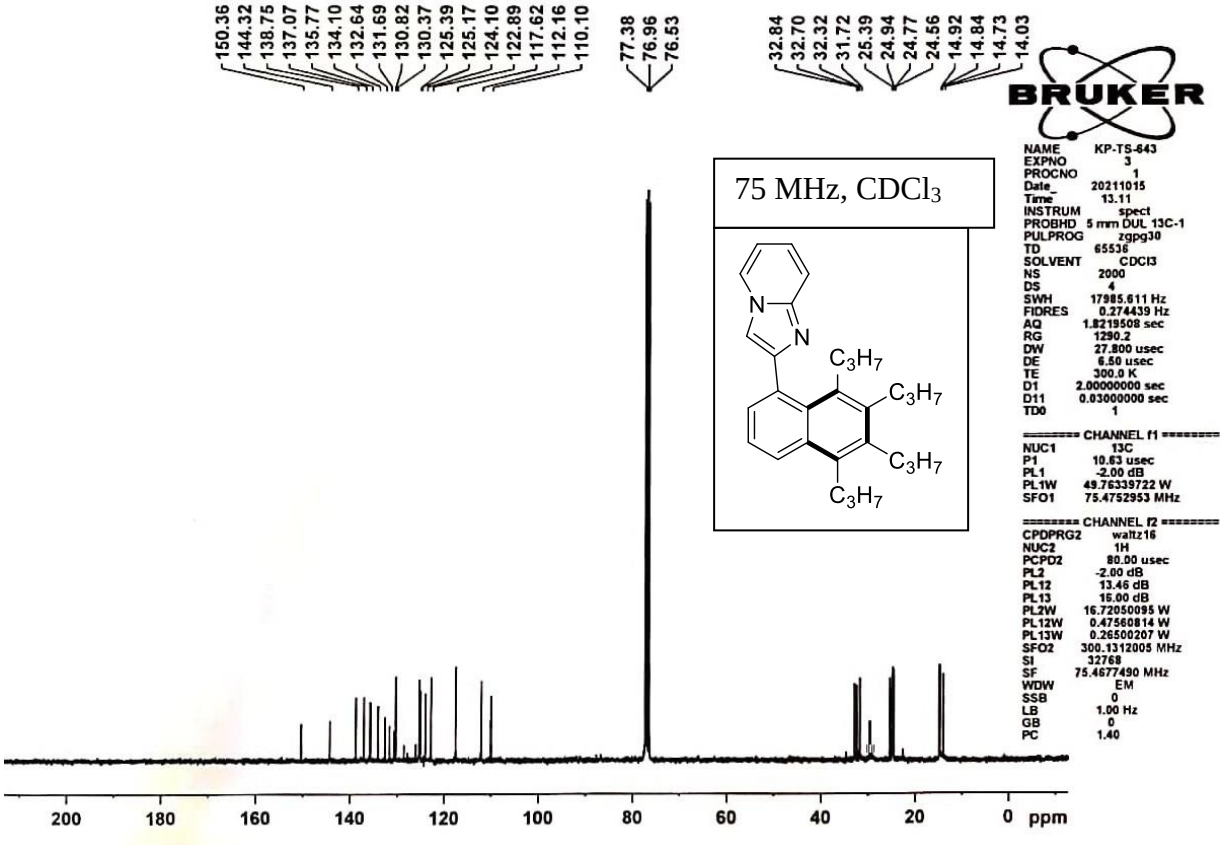


^{1}H and ^{13}C NMR spectra of compound **(5j)**

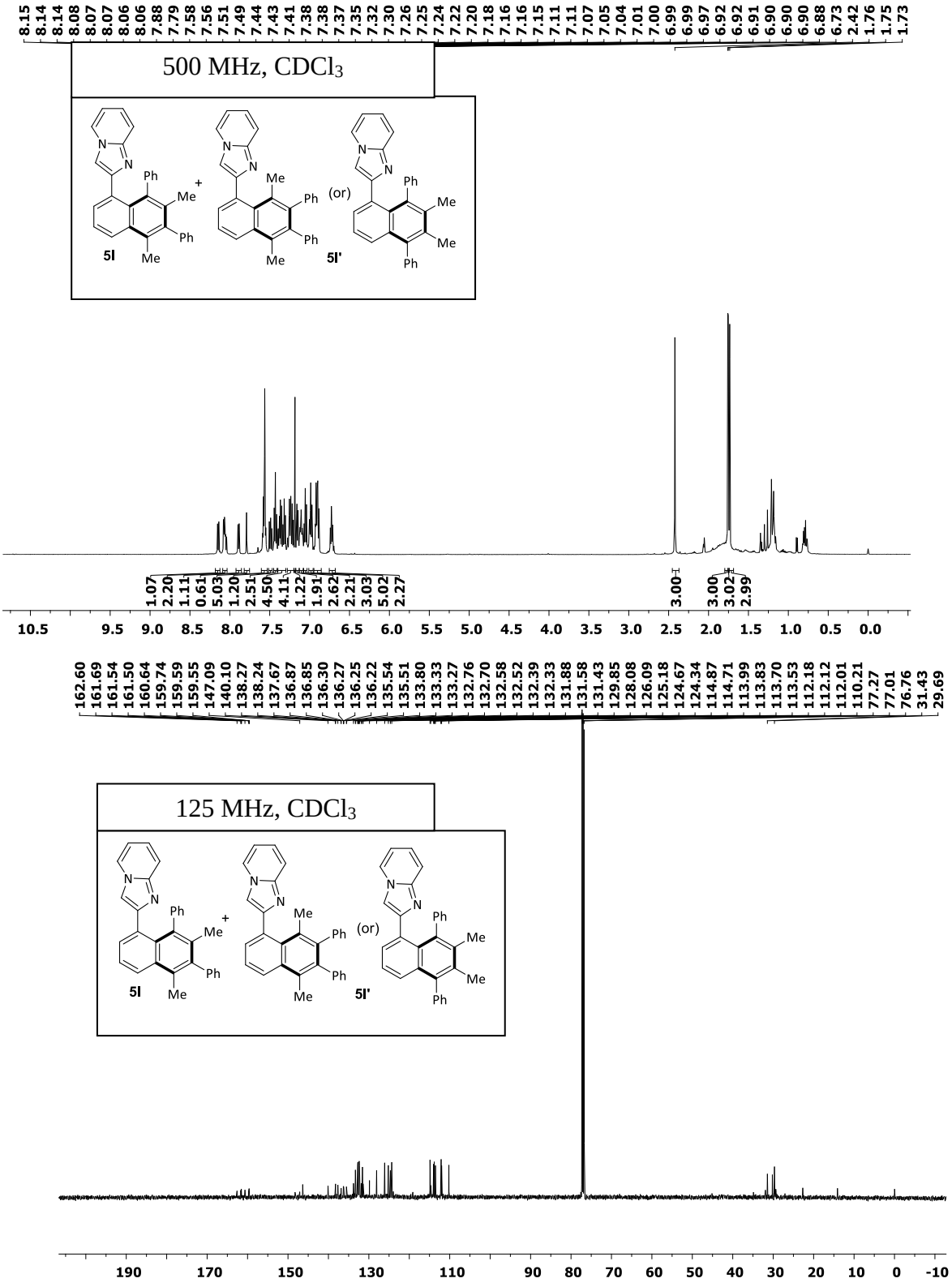


^{1}H and ^{13}C NMR spectra of compound **(5k)**

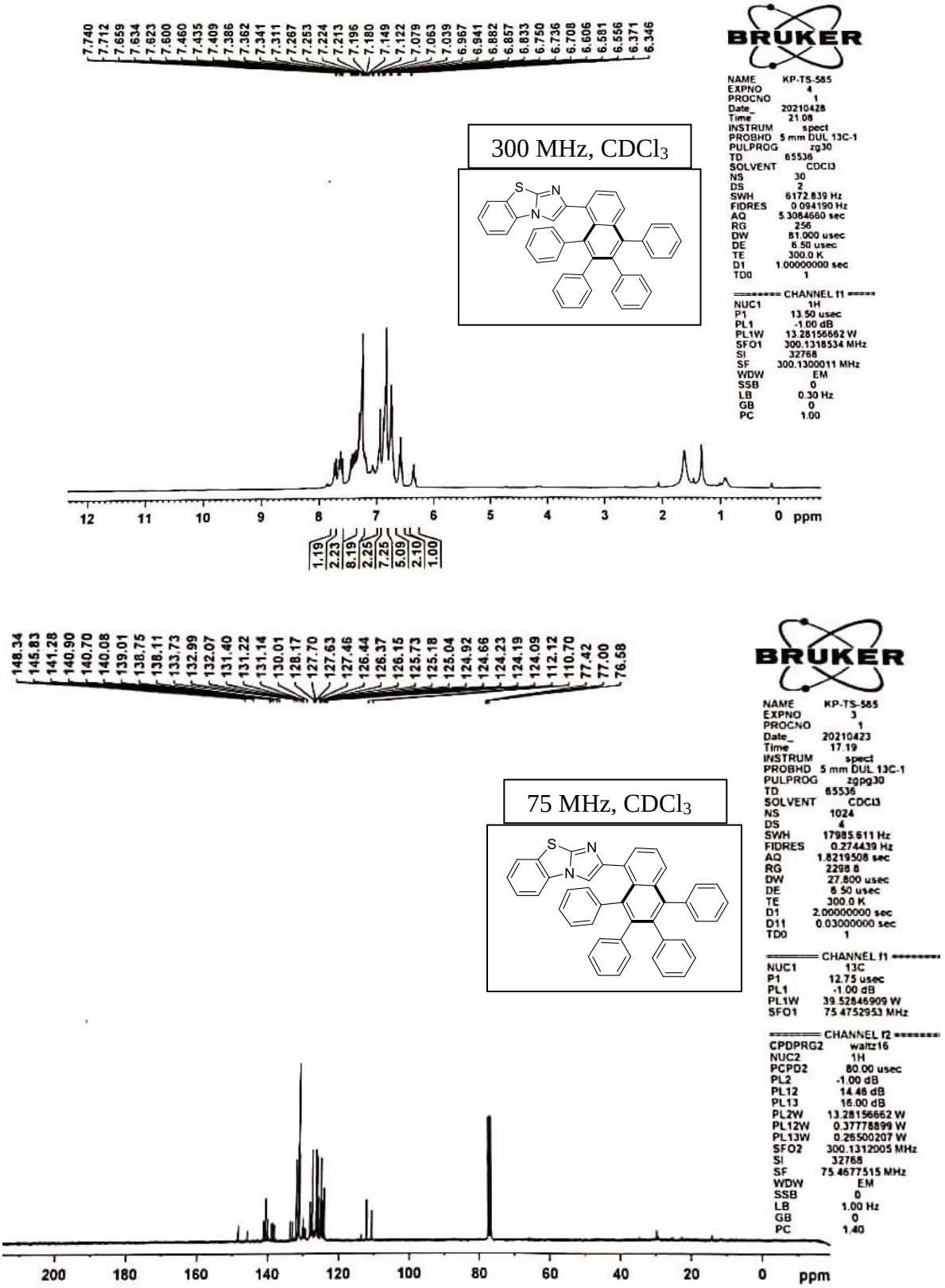




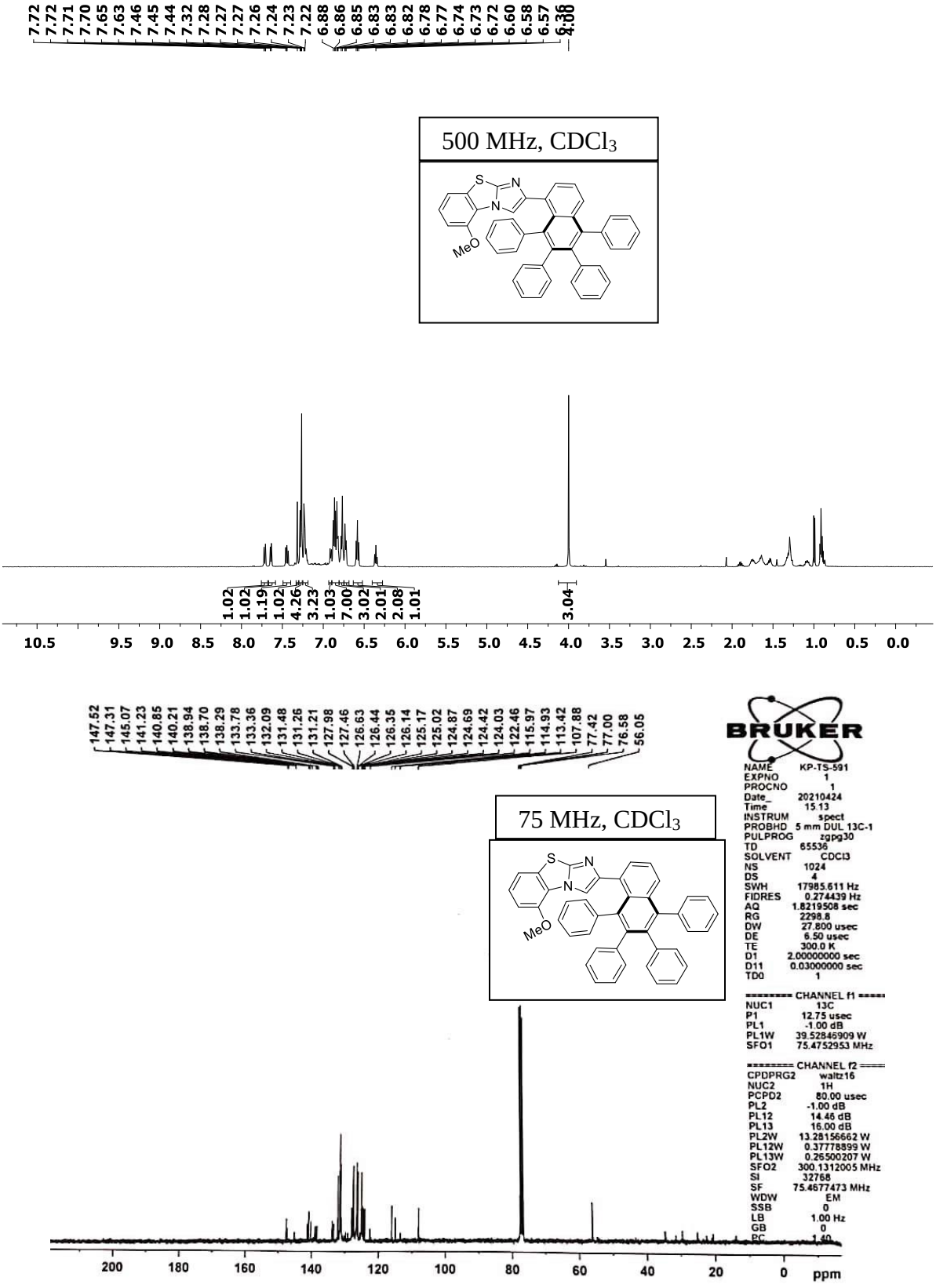
2-(5,7-Dimethyl-6,8-diphenylnaphthalen-1-yl)imidazo[1,2-a]pyridine (5l) and 2-(5,8-dimethyl-6,7-diphenylnaphthalen-1-yl)imidazo[1,2-a]pyridine (5l')



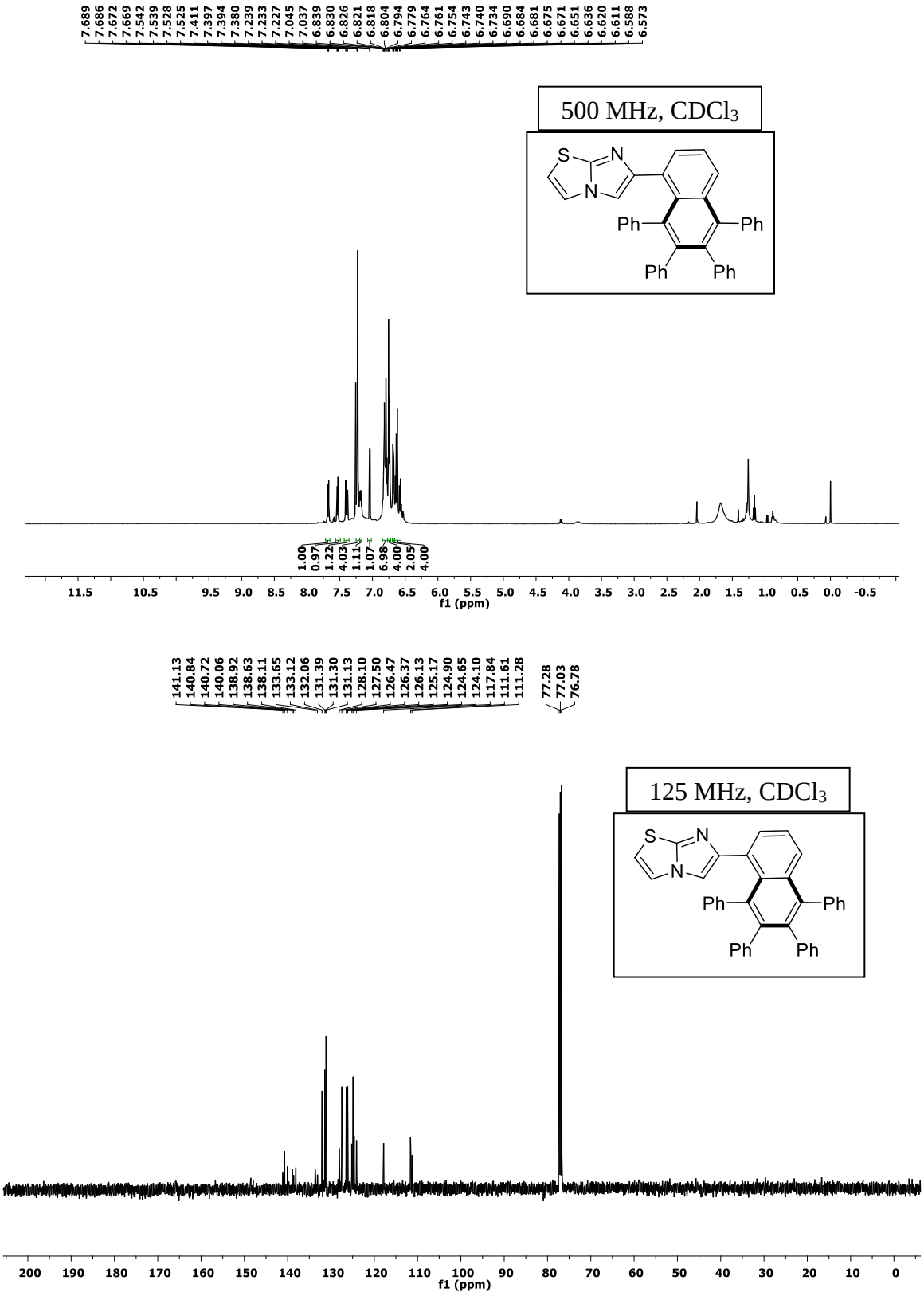
^{1}H and ^{13}C NMR spectra of compound **(7a)**



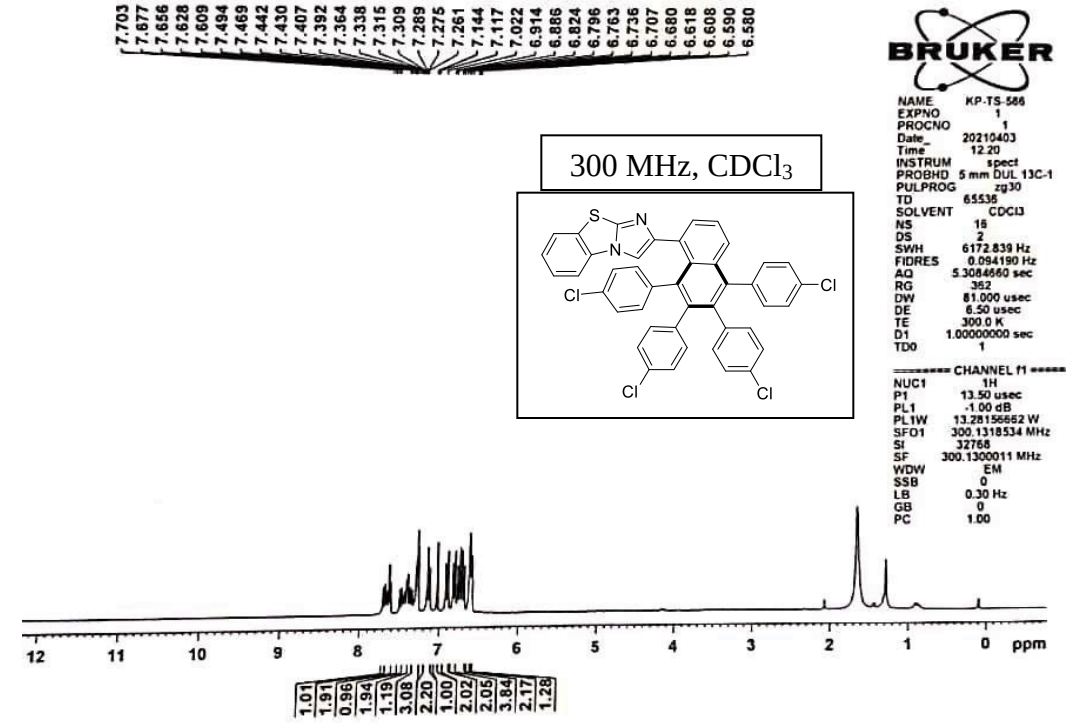
^{1}H and ^{13}C NMR spectra of compound **(7b)**

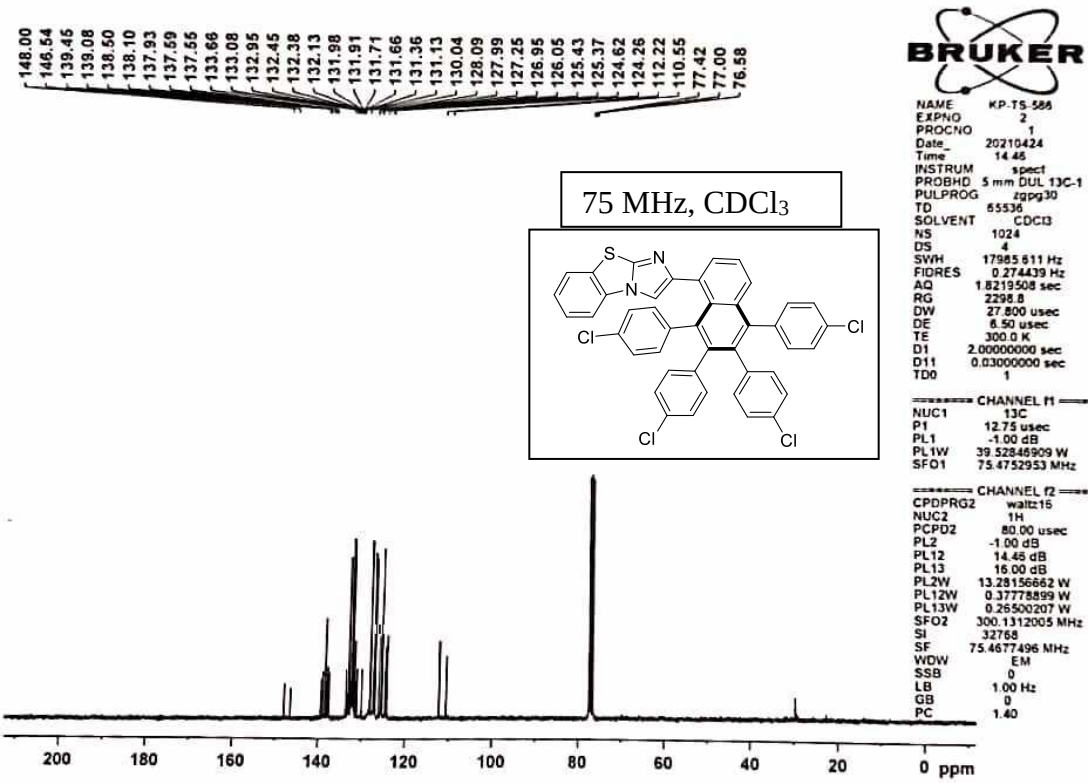


^{1}H and ^{13}C NMR spectra of compound **(7c)**

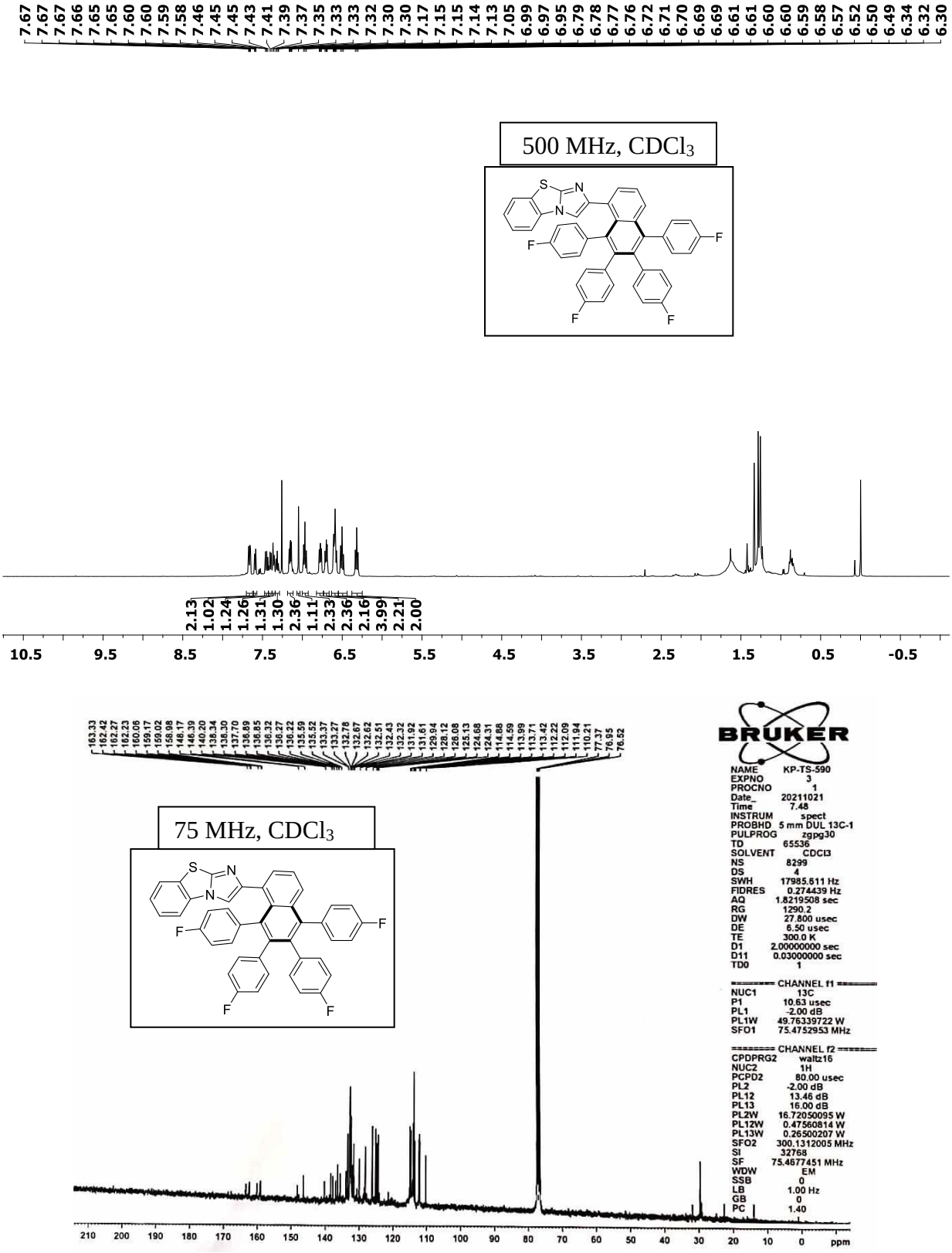


^{1}H and ^{13}C NMR spectra of compound **(7d)**

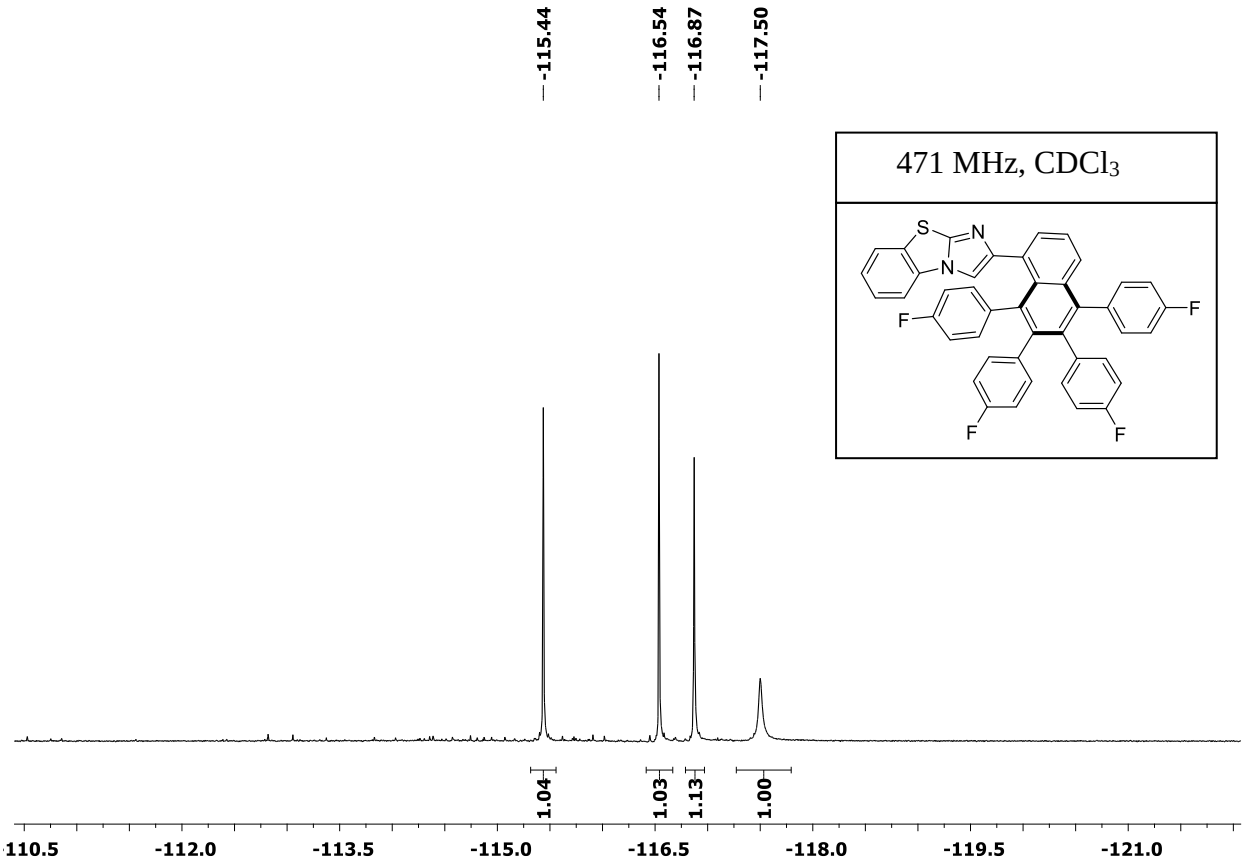




^{1}H and ^{13}C NMR spectra of compound **(7e)**



^{19}F NMR spectra of (7e)



^{1}H and ^{13}C NMR spectra of compound **(9a)**