Supporting Information

Dinuclear Palladium(II) Complexes of N-(imidazo[1,5-*a*]pyridin-1-yl)picolinimidamides: Highly Active Catalyst for C – C and C – P Bond Formation

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General Methods and Instrumentation

The solvents were purchased from commercial sources, chemicals used in this report were of reagent grade, obtained from Sigma-Aldrich and TCI, used without any further purification unless otherwise stated. Palladium catalysts $Pd(PPh_3)_2Cl_2$ and $Pd(dba)_2$ were purchased from TCI. The catalytic products were purified by preparative thin layer chromatography using ethyl acetate and hexane as eluting agents. Fourier Transform Infrared (FT-IR) measurements were recorded by using a Perkin–Elmer attenuated total reflection infrared (ATR-IR) spectrophotometer (4000–400 cm^{-1}). NMR spectra were recorded in $CDCl_3$ and DMSO-d_6 on Bruker 400MHz, 500 MHz, and 600 MHz instruments. The chemical shift values (δ) (ppm) and the spin–spin coupling constant (J) (Hz) were determined by comparing them to tetramethylsilane (TMS), a standard internal reference with a value of zero ppm. FESEM images of the dry powder sample were taken on a Sigma 300 FESEM instrument (Carl Zeiss). Perkin Elmer Lambda-35 UV–visible spectrometer was used to record absorption spectra with quartz cuvettes of 1 cm path length. Electrospray ionization high resolution mass (ESI-HRMS) spectra were recorded on an Agilent MS Model G6546A (Serial Number SG2242E201) Q-TOF mass spectrometer and the simulated spectra were calculated by using MestReNova software. All known compounds were characterized by using NMR spectroscopy and compared with the literature.

General procedure for synthesis of ligands

The ligands were synthesized following a reported procedure with some modification. The corresponding aldehyde, 2-cyanopyridine, and ammonium acetate in 1:2:2 ratio was heat at 100 °C in an oil-bath for 12 h. To the resultant red gummy oil 25 mL of water was added with mechanical stirring for next 12 h. Then, 50 mL dichloromethane was added to the mixture, organic layer was collected and the solid obtained was dried in vacuum over fused $CaCl_2$. The products were isolated as crystalline fibrous solid after column chromatography using silica gel (60-120 mesh) and ethyl acetate/hexane (1:9) as eluent.

N-(3-(2-methoxyphenyl)imidazo[1,5-*a*]pyridin-1-yl)picolinimidamide **(L1H)**

2-methoxybenzaldehyde (0.68 g, 0.005 mol) and 2-cyanopyridine (1.04 g, 0.01 mol) was used. Yield: (1.37 g) 80%. Anal. calcd for $C_{20}H_{17}N_5O$: C, 69.96%; H, 4.99%; N, 20.40%; found: C, 70.11%; H, 5.05%; N, 20.47. ATR-IR (neat, cm^{-1}): 3448, 2922, 2853, 1745, 1616, 1563, 1462, 1380, 1309, 1269, 1238, 1162, 1105, 1077, 956, 759, 729, 747, 711. 466, 427. ^{1}H NMR (400 MHz,

DMSO-d_6) δ 9.28 (s, 1H), 8.64 (d, J = 7.9 Hz, 1H), 8.58 (d, J = 5.5 Hz, 1H), 7.92 (d, J = 9.0 Hz, 1H), 7.80 (td, J = 7.8, 1.7 Hz, 1H), 7.68 (dd, J = 7.5, 1.7 Hz, 1H), 7.54 – 7.44 (m, 2H), 7.34 – 7.30 (m, 1H), 7.13 (t, J = 7.9 Hz, 1H), 7.06 (d, J = 8.3 Hz, 1H), 6.69 (dd, J = 9.0, 6.3 Hz, 1H), 6.54 (t, J = 6.8 Hz, 1H), 3.83 (s, 3H), 1.26 (hexane residue). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 157.4, 153.1, 150.1, 148.0, 140.2, 136.4, 132.6, 130.9, 130.5, 125.3, 124.2, 122.5, 121.6, 121.2, 119.7, 119.0, 116.5, 113.2, 111.5, 55.7. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 355 (14700), 399 (15700), 417 (15900), 443 (10600). HRMS (ESI) *m/z* calcd for $(C_{20}H_{17}N_5O+H)^+$: 344.1506; found 344.1510.

N-(3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridin-1-yl)picolinimidamide **(L2H)**
4-methoxybenzaldehyde (0.68 g, 0.005 mol) and 2-cyanopyridine (1.04 g, 0.01 mol) was used. Yield: (1.44 g) 84%. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 357 (18400), 400(16000), 425 (15260). ATR-IR, NMR and HRMS data were matched well with the literature.

N-(3-(2-chlorophenyl)imidazo[1,5-*a*]pyridin-1-yl)picolinimidamide **(L3H)**
2-chlorobenzaldehyde (0.70 g, 0.005 mol) and 2-cyanopyridine (1.04 g, 0.01 mol) was used. Yield: (1.51 g) 87%. Anal. calcd for Chemical Formula: $C_{19}H_{14}ClN_5$: C, 65.61%; H, 4.06%; N, 20.14%; found: C, 65.72%; H, 4.10%; N, 20.23. ATR-IR (neat, cm^{-1}): 3460, 2923, 2853, 1738, 1616, 1562, 1467, 1440, 1382, 1324, 1235, 1133, 1033, 992, 727, 709, 453, 420. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.18 (s, 1H), 8.62 (d, J = 8.0 Hz, 1H), 8.58 (d, J = 4.8 Hz, 1H), 7.94 (d, J = 9.0 Hz, 1H), 7.80 (td, J = 7.8, 1.7 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.59 – 7.51 (m, 2H), 7.45 – 7.41 (m, 2H), 7.35 – 7.30 (m, 1H), 6.77 – 6.69 (m, 1H), 6.60 (t, J = 7.3 Hz, 1H), 1.26 (hexane residue). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 152.9, 150.8, 148.1, 140.1, 136.5, 134.3, 133.0, 130.5, 130.4, 130.3, 129.7, 127.2, 125.0, 124.3, 121.6, 121.4, 119.4, 117.0, 114.1. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 355 (18500), 400 (16100), 427 (15000), 452 (9800). HRMS (ESI) *m/z* calculated for $(C_{19}H_{14}ClN_5+H)^+$: 348.1011; found 348.1026.

N-(3-(4-methylphenyl)imidazo[1,5-*a*]pyridin-1-yl)picolinimidamide **(L4H)**
4-methylbenzaldehyde (0.6 g, 0.005 mol) and 2-cyanopyridine (1.04 g, 0.01 mol) was used. Yield: (1.26 g) 77%. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 274 (13330), 361 (12870), 401 (10870), 425 (9900). ATR-IR, NMR and HRMS data were matched well with the literature.

N-(3-(4-bromophenyl)imidazo[1,5-*a*]pyridin-1-yl)picolinimidamide **(L5H)**

4-bromobenzaldehyde (0.92 g, 0.005 mol) and 2-cyanopyridine (1.04 g, 0.01 mol) was used. Yield: (1.41 g) 72%. Anal. calcd for Chemical Formula: $C_{19}H_{14}BrN_5$: C, 58.18%; H, 3.60%; N, 17.85%; found: C, 58.26%; H, 3.67%; N, 17.91. ATR-IR (neat, cm^{-1}): 3434, 2922, 2852, 1744, 1620, 1528, 1494, 1466, 1371, 1305, 1243, 1075, 994, 948, 832, 798, 709, 502, 470, 442. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 236 (18600), 375 (15670), 399(14700), 424 (11830). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.21 (s, 1H), 8.62 – 8.58 (m, 2H), 8.16 (d, *J* = 7.2 Hz, 1H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.80 (td, *J* = 7.6, 1.7 Hz, 1H), 7.73 (d, *J* = 8.6 Hz, 2H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.42 (s, 1H), 7.36 – 7.31 (m, 1H), 6.71 – 6.66 (m, 1H), 6.62 (td, *J* = 6.9, 6.5, 1.3 Hz, 1H), 1.26 (hexane residue). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 161.87, 149.59, 148.39, 137.65, 133.72, 132.40, 129.46, 128.95, 127.42, 126.57, 122.87, 122.49, 122.25, 121.62, 120.76, 118.02, 114.25. HRMS (ESI) *m/z* calculated for $(C_{19}H_{14}BrN_5+H)^+$: 392.0505; found 392.0514.

General procedure for synthesis of palladium complexes:

The dinuclear palladium complexes were synthesized by a general procedure. For this, Palladium dichloride (88 mg, 0.5 mmol) was taken in 10 mL acetonitrile and was heated till all $PdCl_2$ dissolved. To the squash colour hot solution, corresponding ligand (**L1H** – **L3H**) (0.5 mmol) was added resulting a deep red/orange colour solution. The mixture was left at ambient temperature with continuous stirring for 12 hours. The solvent was removed, solids were washed with diethyl ether, and dried in vacuo to afford the desired dinuclear palladium complexes (**1** – **3**). Following the similar method, solids obtained from the reaction of $PdCl_2$ with **L4H** and **L5H** were dissolved it methanol, KPF_6 was then added and stirred for about 2 hours at room temperature. Orange solids were precipitated out, filtered, washed with diethyl ether, and dried in vacuo to afford the dinuclear palladium complexes **4** and **5**.

$[Pd_2(\mathbf{L1H})_2Cl_2]Cl_2$ (**1**)

Following the general procedure, complex **1** was synthesized from the reaction of $PdCl_2$ and **L1H**. Yield: (0.385 g) 74%. Anal. calcd for $C_{40}H_{34}Cl_4N_{10}O_2Pd_2$: C, 46.13%; H, 3.29%; N, 13.45%; found: C, 46.20%; H, 3.31%; N, 13.52. ATR-IR (neat, cm^{-1}): 2924, 1720, 1645, 1566, 1454, 1250, 1017, 751, 628, 432. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 304 (28000), 385 (11800), 440 (6000). ^{1}H NMR (400 MHz, DMSO-*d*6) δ 9.56 (s, 2H), 9.14 (d, *J* = 5.1 Hz, 2H), 8.61 (s, 2H), 8.57 – 8.50 (m, 4H), 8.46 (t, *J* = 7.7 Hz, 2H), 7.98 (t, *J* = 6.7 Hz, 2H), 7.62 (t, *J* = 7.1 Hz, 2H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.09 (d, *J* = 8.6 Hz, 2H), 6.96 (s, 4H), 6.80 (dt, *J* = 7.4, 3.7 Hz, 2H),

3.34 (s, 6H), 2.87 (DMF-CH_3), 2.71 (DMF-CH_3), 1.26 (hexane residue). ^{13}C NMR (151 MHz, DMSO-d_6) δ 165.00, 157.53, 152.08, 151.73, 142.64, 133.47, 132.99, 132.31, 130.41, 128.57, 127.79, 126.46, 124.15, 123.02, 120.99, 116.37, 115.52, 114.01, 112.17, 56.32. HRMS (ESI) *m/z* calculated for $[C_{40}H_{34}Cl_4N_{10}O_2Pd_2–2Cl]^{2+}$: 485.0155, found 485.0128 and for $[C_{40}H_{34}Cl_4N_{10}O_2Pd_2–2Cl–H]^{+}$: 969.0238, found 969.0178.

$[Pd_2(\mathbf{L2H})_2Cl_2]Cl_2$ (**2**)

Following the general procedure, complex **2** was synthesized from the reaction of $PdCl_2$ and **L2H**. Yield: (0.375 g) 72%. Anal. calcd for $C_{40}H_{34}Cl_4N_{10}O_2Pd_2$: C, 46.13%; H, 3.29%; N, 13.45%; found: C, 46.19%; H, 3.35%; N, 13.50. ATR-IR (neat, cm^{-1}): 3084, 1651, 1609, 1557, 1456, 1252, 1177, 1025, 839, 795, 748, 575, 523, 440. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 311 (19300), 352 (10800), 428 (7600). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 2H), 9.09 (d, *J* = 5.0 Hz, 2H), 8.77 (s, 2H), 8.66 (d, *J* = 7.3 Hz, 2H), 8.51 (t, *J* = 7.5 Hz, 2H), 7.97 (dt, *J* = 15.8, 7.4 Hz, 4H), 7.62 (d, *J* = 8.5 Hz, 4H), 7.32 (d, *J* = 9.2 Hz, 2H), 7.17 (d, *J* = 8.6 Hz, 4H), 7.04 – 6.95 (m, 2H), 6.80 (t, *J* = 6.7 Hz, 2H), 3.86 (s, 6H), 2.88 (DMF-CH_3), 2.72 (DMF-CH_3). ^{13}C NMR (151 MHz, DMSO-d_6) δ 165.32, 162.62, 161.06, 152.01, 151.38, 142.34, 134.47, 131.14, 130.10, 128.63, 126.25, 122.83,121.86, 117.34, 117.17, 116.27, 115.04, 55.68. HRMS (ESI) *m/z* calculated for $[C_{40}H_{34}Cl_4N_{10}O_2Pd_2–2Cl]^{2+}$: 485.0155, found 485.0130; $[C_{40}H_{34}Cl_4N_{10}O_2Pd_2–2Cl–H]^{+}$: 969.0238, found 969.0182.

$[Pd_2(\mathbf{L3H})_2Cl_2]Cl_2$ (**3**)

Following the general procedure, complex **3** was synthesized from the reaction of $PdCl_2$ and **L3H**. Yield: (0.446 g) 85%. Anal. calcd for $C_{38}H_{28}Cl_6N_{10}Pd_2$: C, 43.46%; H, 2.69%; N, 13.34%; found: C, 43.52%; H, 2.71%; N, 13.42. ATR-IR (neat, cm^{-1}): 3442, 1738, 1626, 1598, 1450, 1354, 1290, 1055, 745, 681, 509, 424. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 321 (20600), 366 (14300), 424 (7890). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.20 (d, *J* = 5.1 Hz, 2H), 8.76 (d, *J* = 7.6 Hz, 2H), 8.06 (d, *J* = 7.7 Hz, 2H), 7.99 (t, *J* = 7.6 Hz, 2H), 7.54 – 7.51 (m, 2H), 7.50 – 7.47 (m, 2H), 7.47 – 7.44 (m, 2H), 7.34 (d, *J* = 7.4 Hz, 2H), 7.16 (d, *J* = 9.2 Hz, 2H), 7.08 (d, *J* = 7.2 Hz, 2H), 6.73 (dd, *J* = 8.8, 6.9 Hz, 2H), 6.55 – 6.52 (m, 2H), 1.60 (H_2O). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.44, 153.96, 149.74, 139.88, 136.33, 134.87, 134.30, 132.03, 130.26, 129.26, 127.62, 126.89, 126.45, 126.17, 122.89, 121.65, 119.79, 119.57, 114.97. HRMS (ESI) *m/z* calculated for

$[C_{38}H_{28}Cl_6N_{10}Pd_2–2Cl]^{2+}$: 489.9652, found 489.9632; $[C_{38}H_{28}Cl_6N_{10}Pd_2–2Cl–H]^{+}$: 978.9231, found 978.9184.

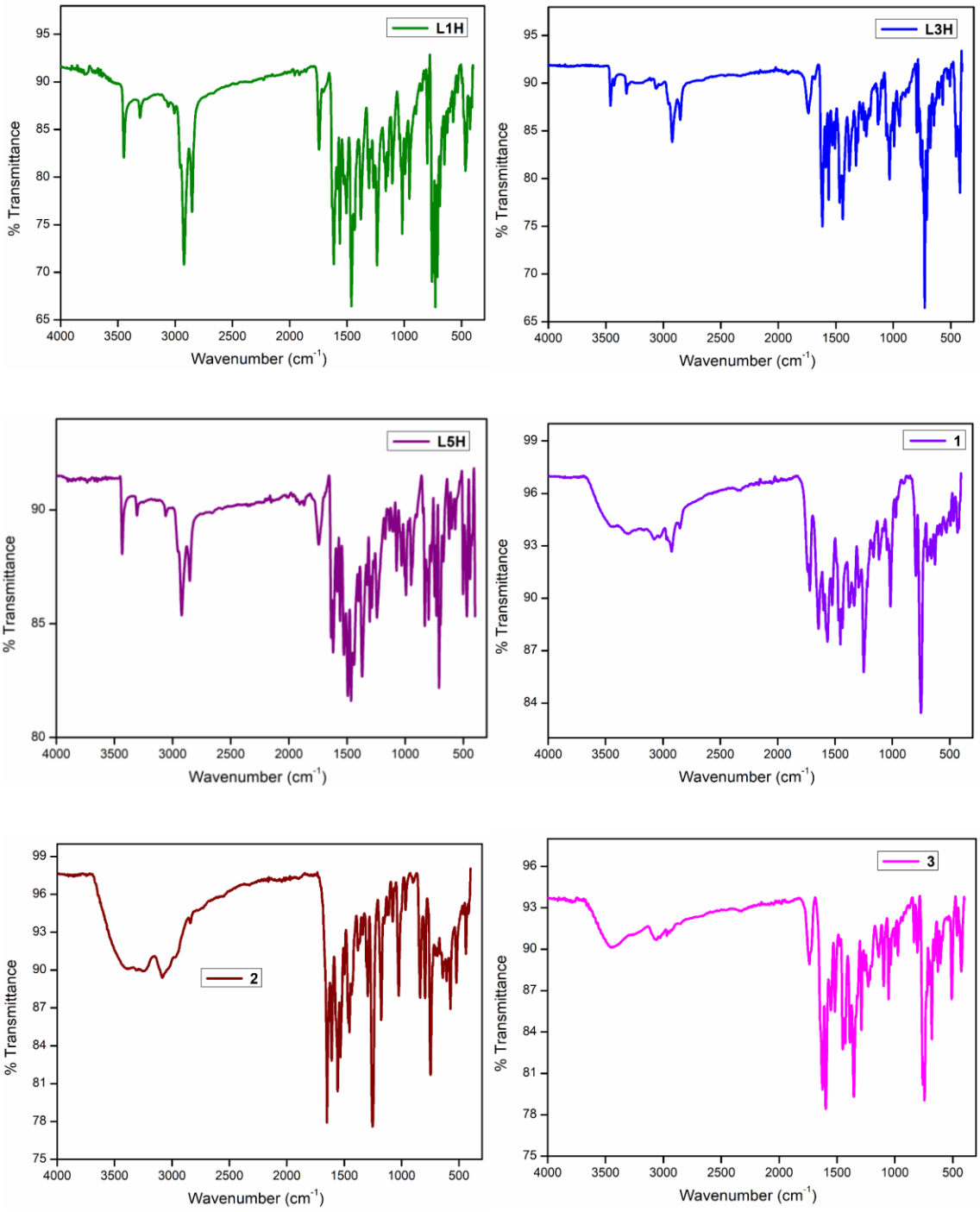
$[Pd_2(\mathbf{L4H})_2Cl_2](PF_6)_2$ (**4**)

Following the general procedure, complex **4** was synthesized from the reaction of $PdCl_2$ and **L4H**. Yield: (0.497 g) 81%. Anal. calcd for $C_{40}H_{34}Cl_2F_{12}N_{10}P_2Pd_2$: C, 39.11%; H, 2.79%; N, 11.40%; found: C, 39.24%; H, 2.81%; N, 11.48. ATR-IR (neat, cm^{-1}): 3086, 1648, 1567, 1384, 1253, 1098, 831, 754, 661, 556, 497, 441. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})):310 (23700), 365 (11500), 426 (8160). ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.66 (s, 2H), 9.10 (d, J = 5.0 Hz, 2H), 8.78 (s, 2H), 8.54 (q, J = 9.1, 7.8 Hz, 4H), 8.01 (t, J = 6.3 Hz, 4H), 7.95 (s, DMF), 7.59 (d, J = 7.9 Hz, 4H), 7.44 (d, J = 7.8 Hz, 4H), 7.35 (d, J = 9.2 Hz, 2H), 6.99 (t, J = 7.8 Hz, 2H), 6.82 (t, J = 6.8 Hz, 2H), 2.89, (s, DMF), 2.73, (s, DMF), 2.43 (s, 6H), 3.36 (H_2O), 2.87 (DMF-CH_3), 2.71 (DMF-CH_3), 2.07 (MeCN), 1.26 (hexane residue). ^{13}C NMR (151 MHz, DMSO-d_6) δ 165.16, 162.33, 151.91, 151.24, 142.22, 140.81, 134.35, 130.02, 129.20, 128.76, 125.99, 122.85, 122.62, 122.22, 121.85, 117.24, 116.21, 35.80, 30.78 (DMF), 21.15 (DMF). ^{31}P NMR (243 MHz, DMSO-d_6) δ -144.19 (sept, J = 710.6 Hz). HRMS (ESI) *m/z* calculated for $[C_{40}H_{34}Cl_2F_{12}N_{10}P_2Pd_2–2PF_6]^{2+}$: 469.0206, found 469.0203; $[C_{40}H_{34}Cl_2F_{12}N_{10}P_2Pd_2–2PF_6–H]^{+}$: 937.0240, found 937.0323.

$[Pd_2(\mathbf{L5H})_2Cl_2]$ $(PF_6)_2$ (**5**)

Following the general procedure, complex **5** was synthesized from the reaction of $PdCl_2$ and **L5H**. Yield: (0.516 g) 76%. Anal. calcd for $C_{38}H_{28}Br_2Cl_2F_{12}N_{10}P_2Pd_2$: C, 33.60%; H, 2.08%; N, 10.31%; found: C, 33.72%; H, 2.14%; N, 10.46. ATR-IR (neat, cm^{-1}): 3074, 1644, 1563, 1521, 1454, 1069, 1009, 965, 795, 747, 496, 434. UV-Vis (λ, nm (Ɛ, M^{-1} cm^{-1})): 328 (21230), 398 (9950), 432 (7700). ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.69 (s, 1H), 9.12 – 9.07 (m, 1H), 8.79 (s, 1H), 8.55 (q, J = 8.1 Hz, 2H), 8.09 (d, J = 7.3 Hz, 1H), 8.02 (t, J = 6.2 Hz, 1H), 7.95 (DMF-CH), 7.86 (d, J = 8.4 Hz, 2H), 7.68 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 9.3 Hz, 1H), 7.10 – 7.04 (m, 1H), 6.89 – 6.83 (m, 1H) , 2.88 (DMF-CH_3), 2.72 (DMF-CH_3). ^{13}C NMR (151 MHz, DMSO-d_6) δ 165.34, 151.97, 151.21, 142.23, 133.05, 132.50, 131.24, 129.95, 129.12, 126.04, 124.50, 124.39, 123.16, 123.09, 122.08, 117.08, 116.47. ^{31}P NMR (162 MHz, DMSO-d_6) δ -144.20 (sept, J = 711.2 Hz). HRMS (ESI) *m/z* calculated for $[C_{38}H_{28}Br_2Cl_2F_{12}N_{10}P_2Pd_2–2PF_6]^{2+}$: 531.8985, found 531.8982; $[C_{38}H_{28}Br_2Cl_2F_{12}N_{10}P_2Pd_2–2PF_6–H]^{+}$: 1066.8217, found 1066.8212.

ATR-IR, NMR, HRMS, UV-Vis spectra and FESEM images of ligands and Pd complexes:



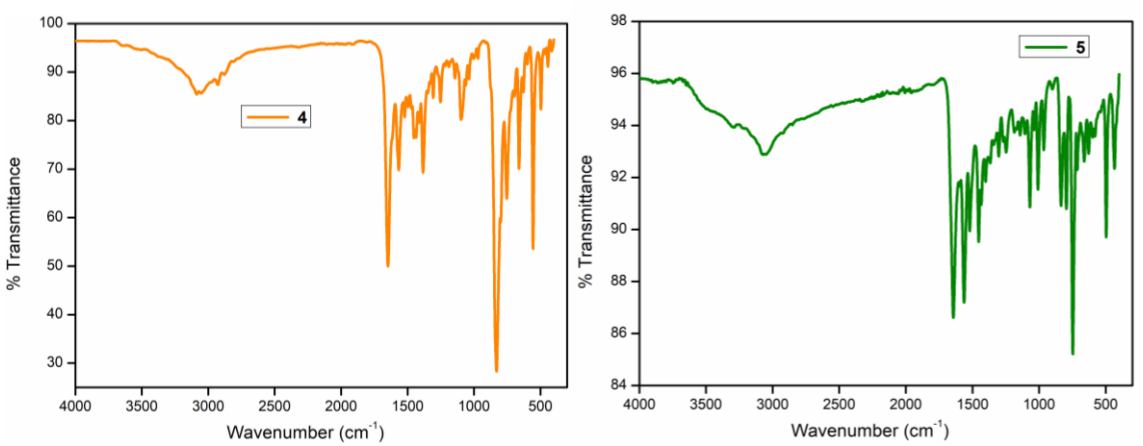
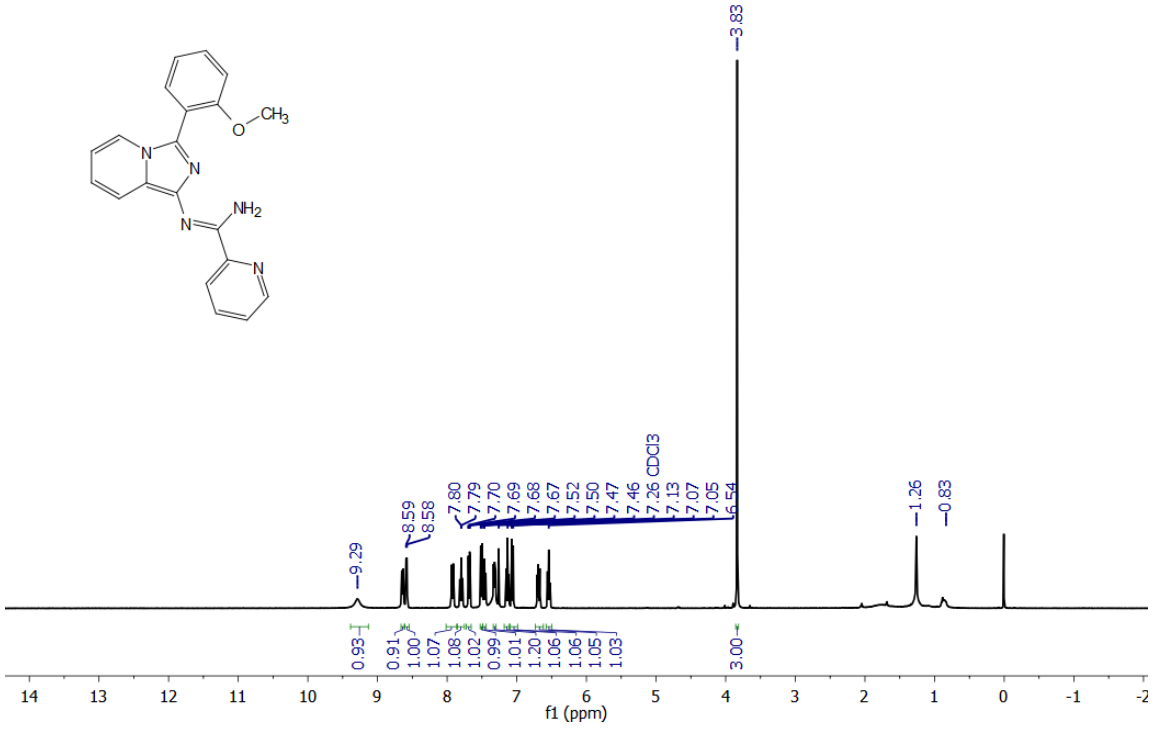


Figure S1. ATR-IR spectra of **L1H**, **L3H**, **L5H** and **1** – **5**.



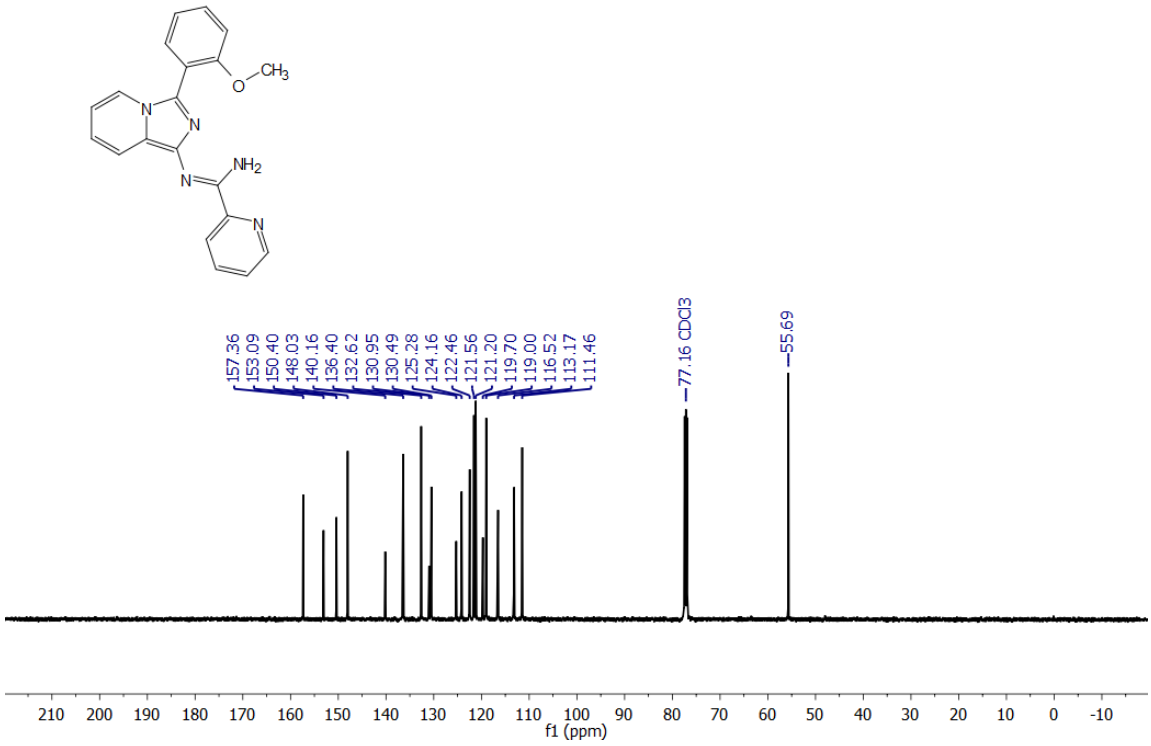
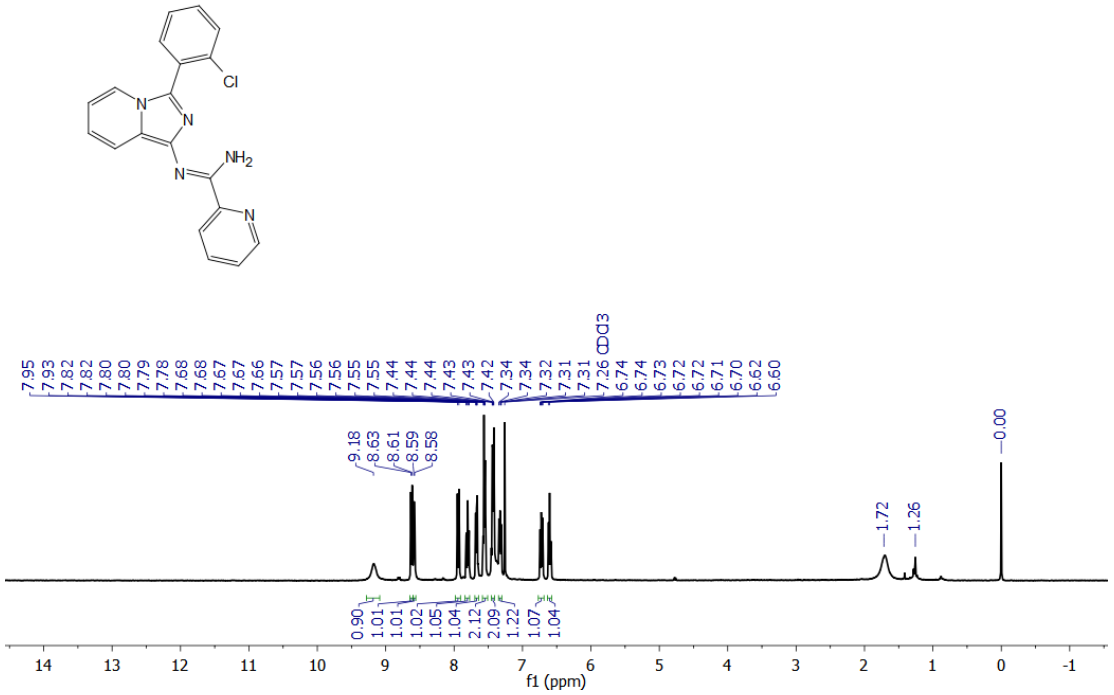


Figure S2. ^{1}H and ^{13}C NMR spectra of **L1H**



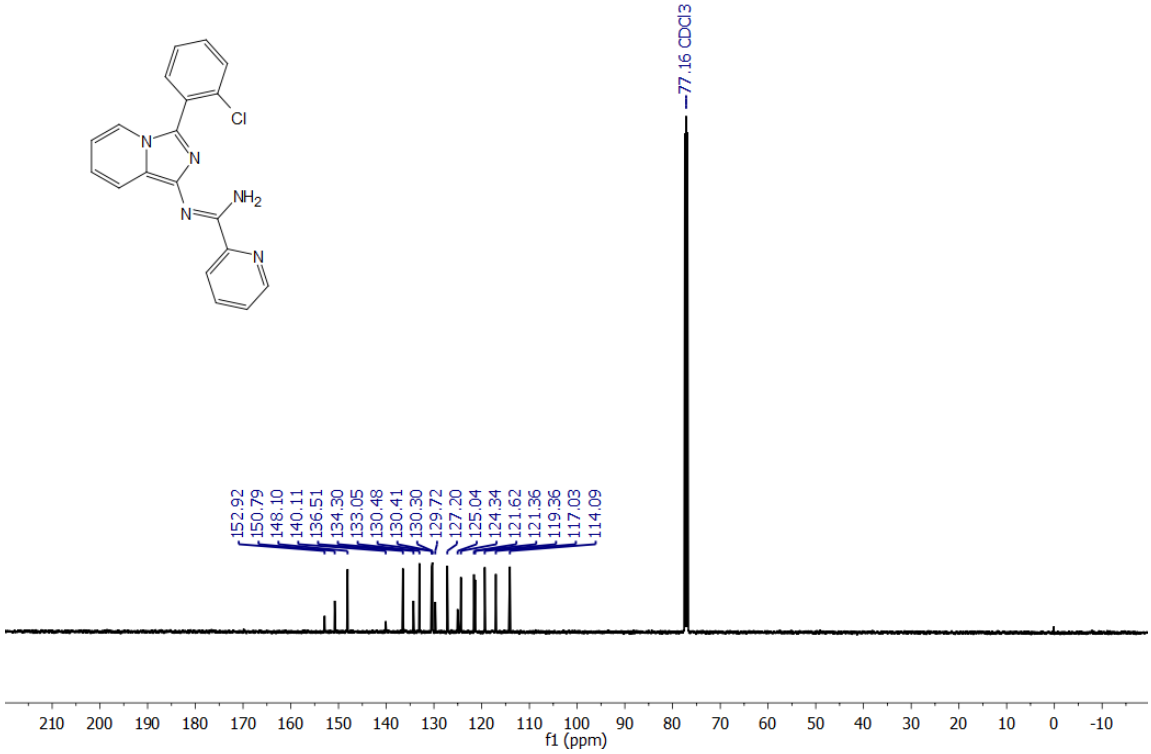
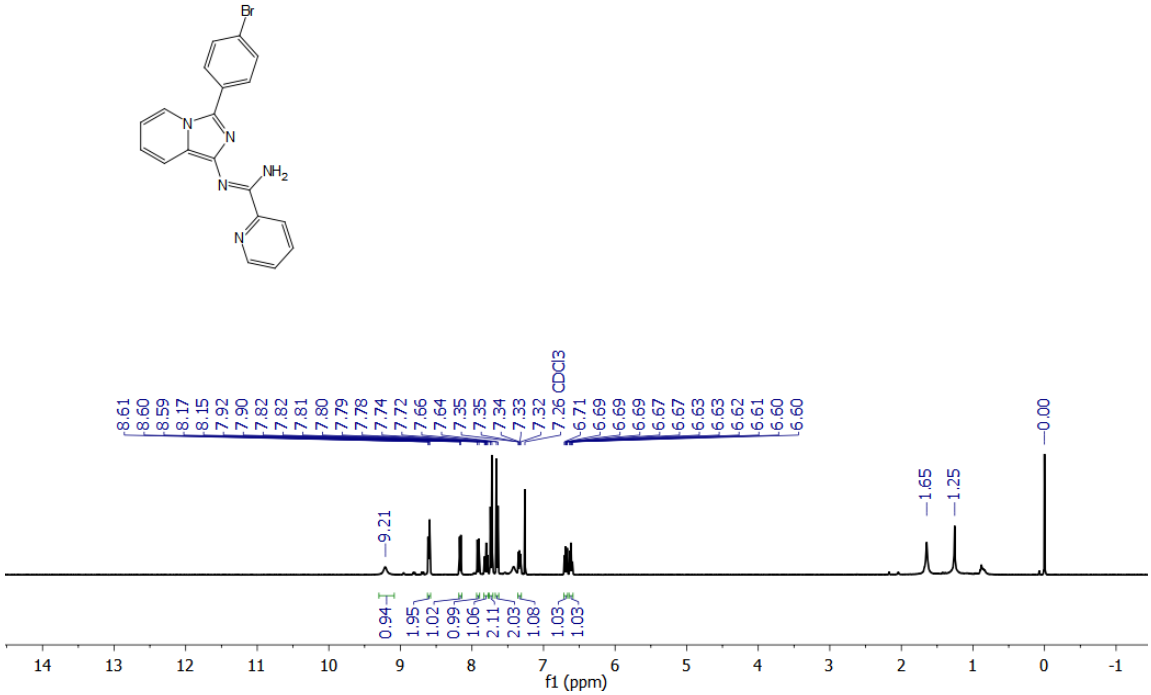


Figure S3. ^{1}H and ^{13}C NMR spectra of **L3H**



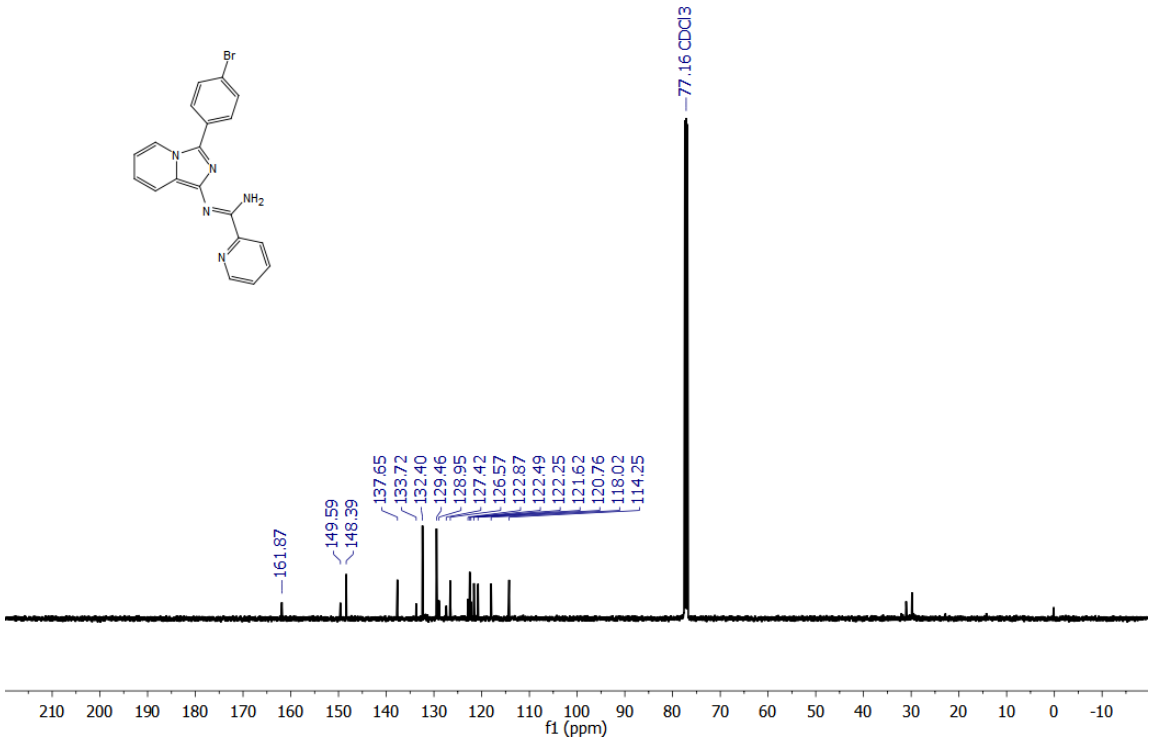
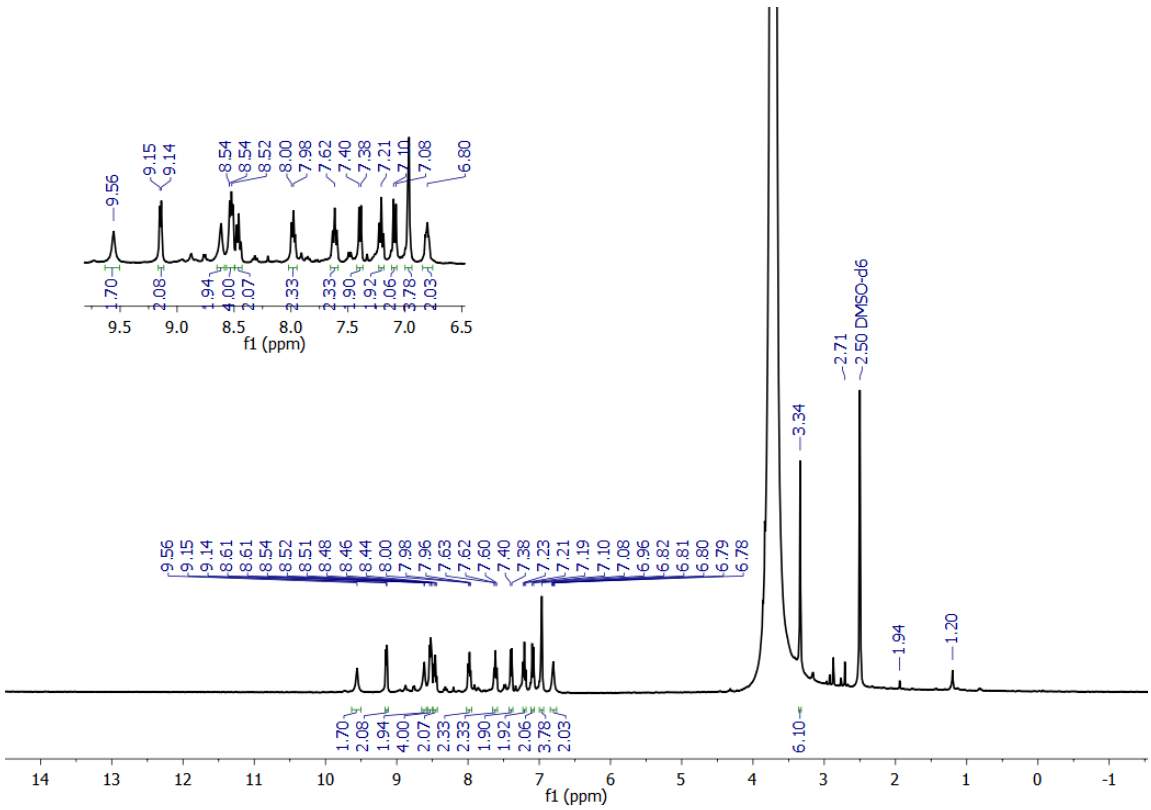


Figure S4. ^{1}H and ^{13}C NMR spectra of **L5H**



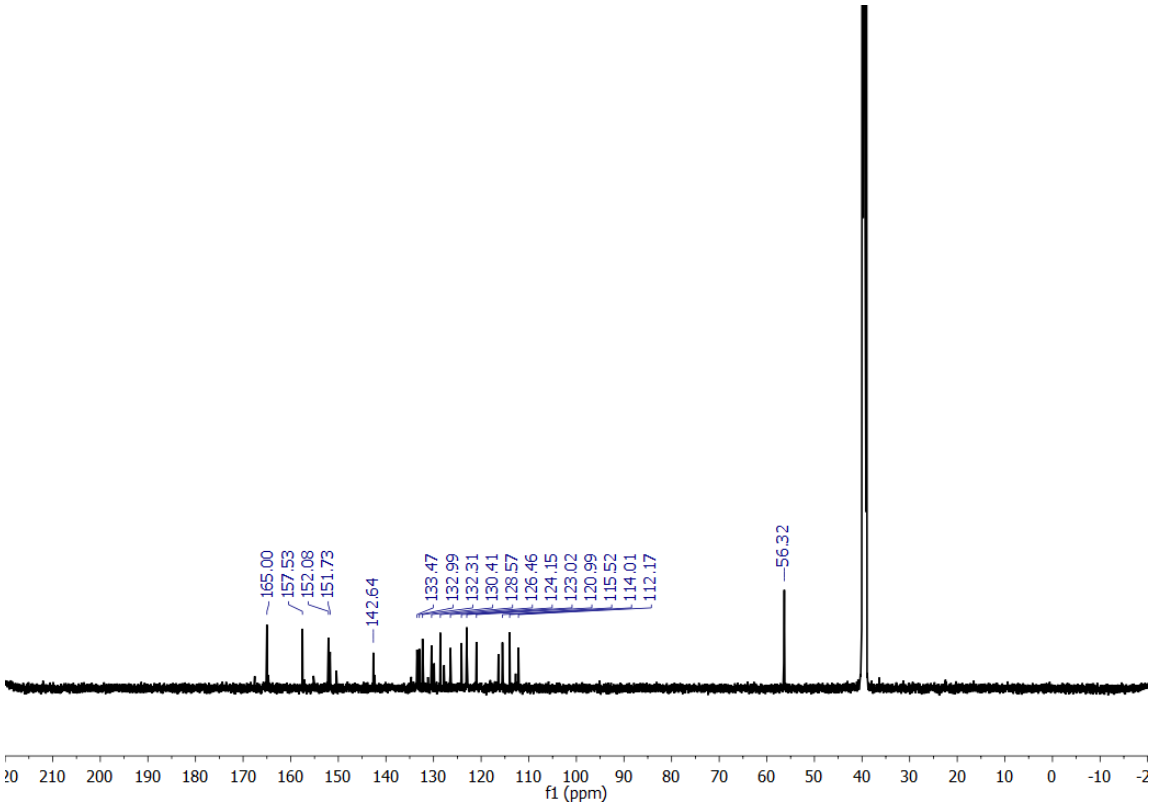
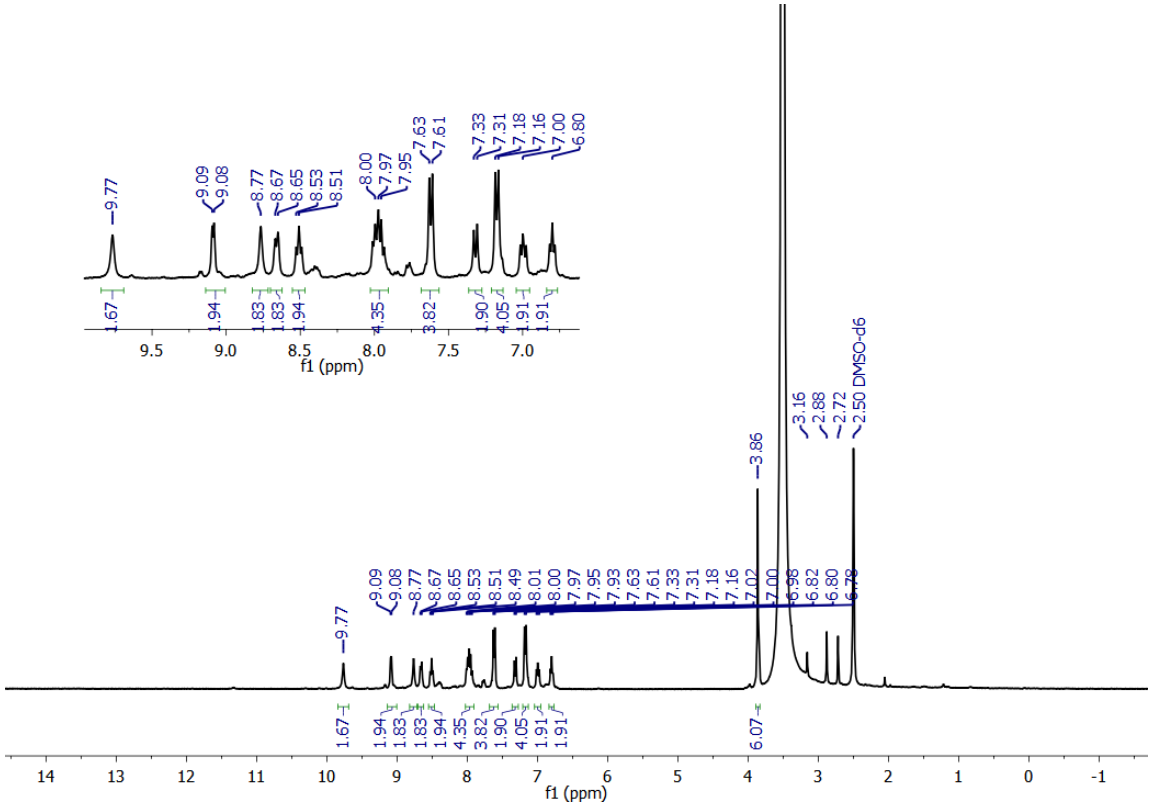


Figure S5. ^{1}H and ^{13}C NMR spectra of **1**



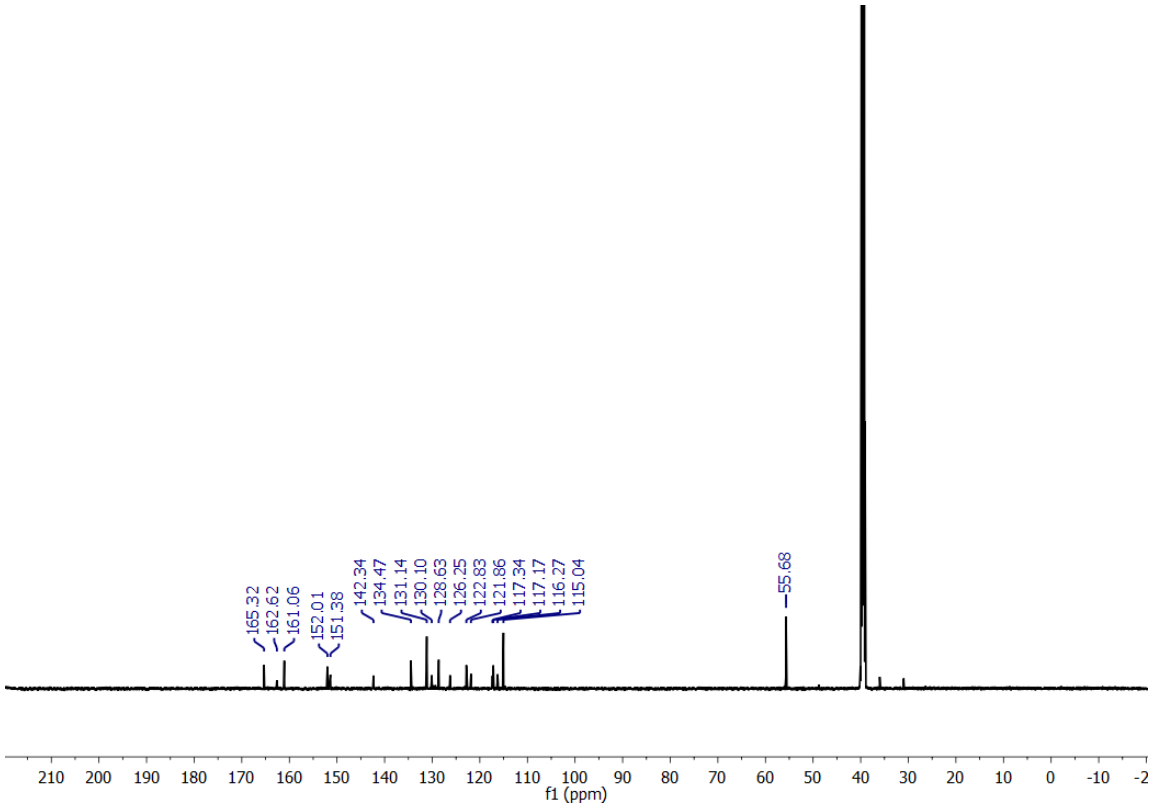
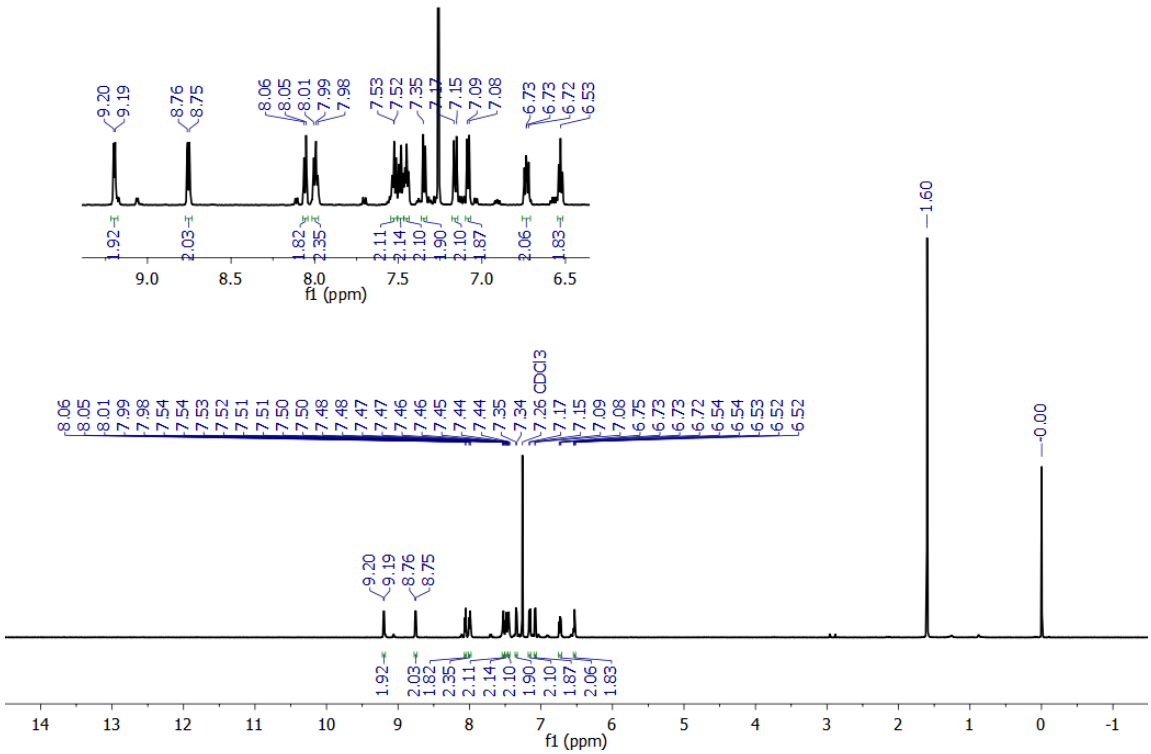


Figure S6. ^{1}H and ^{13}C NMR spectra of **2**



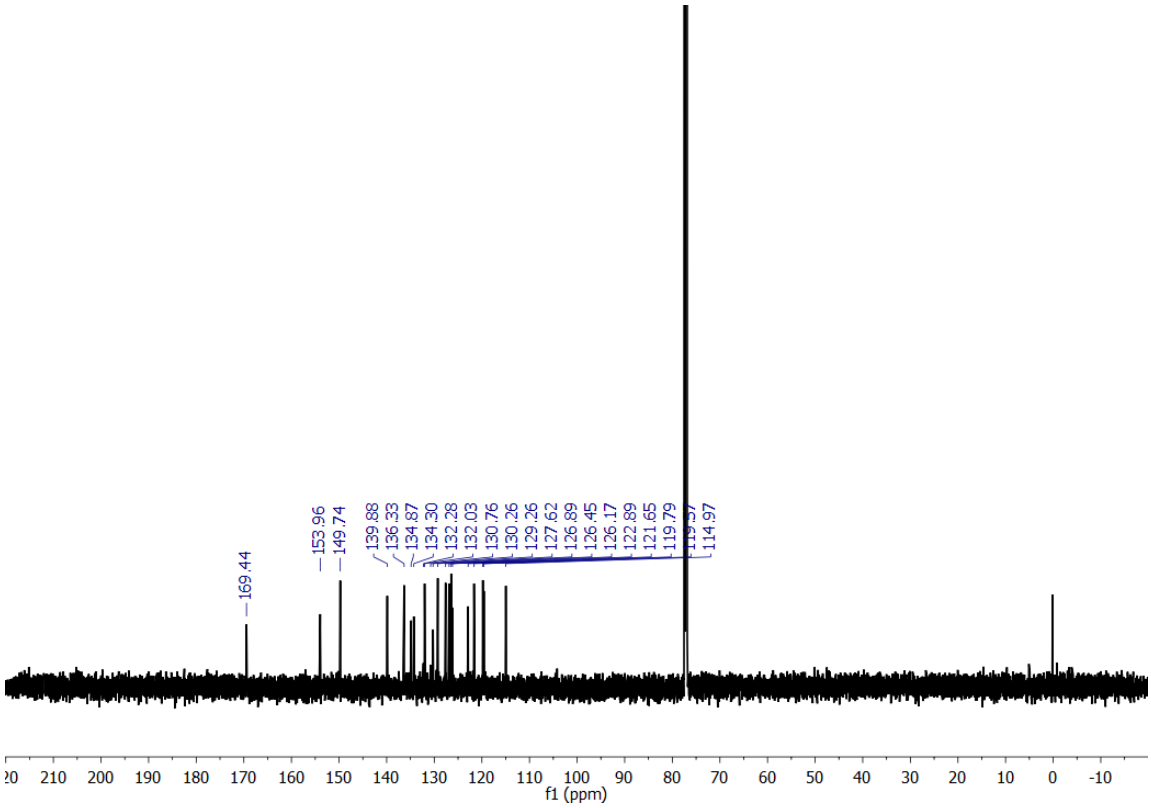
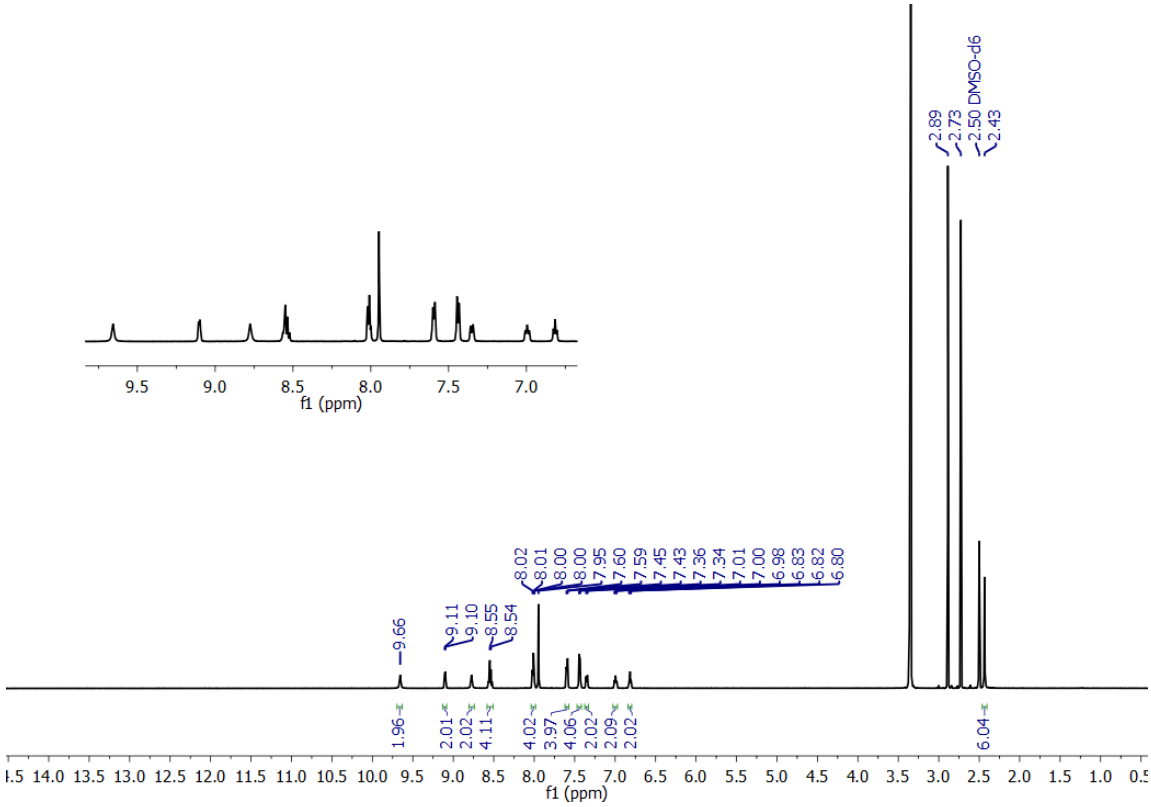


Figure S7. ^{1}H and ^{13}C NMR spectra of **3**



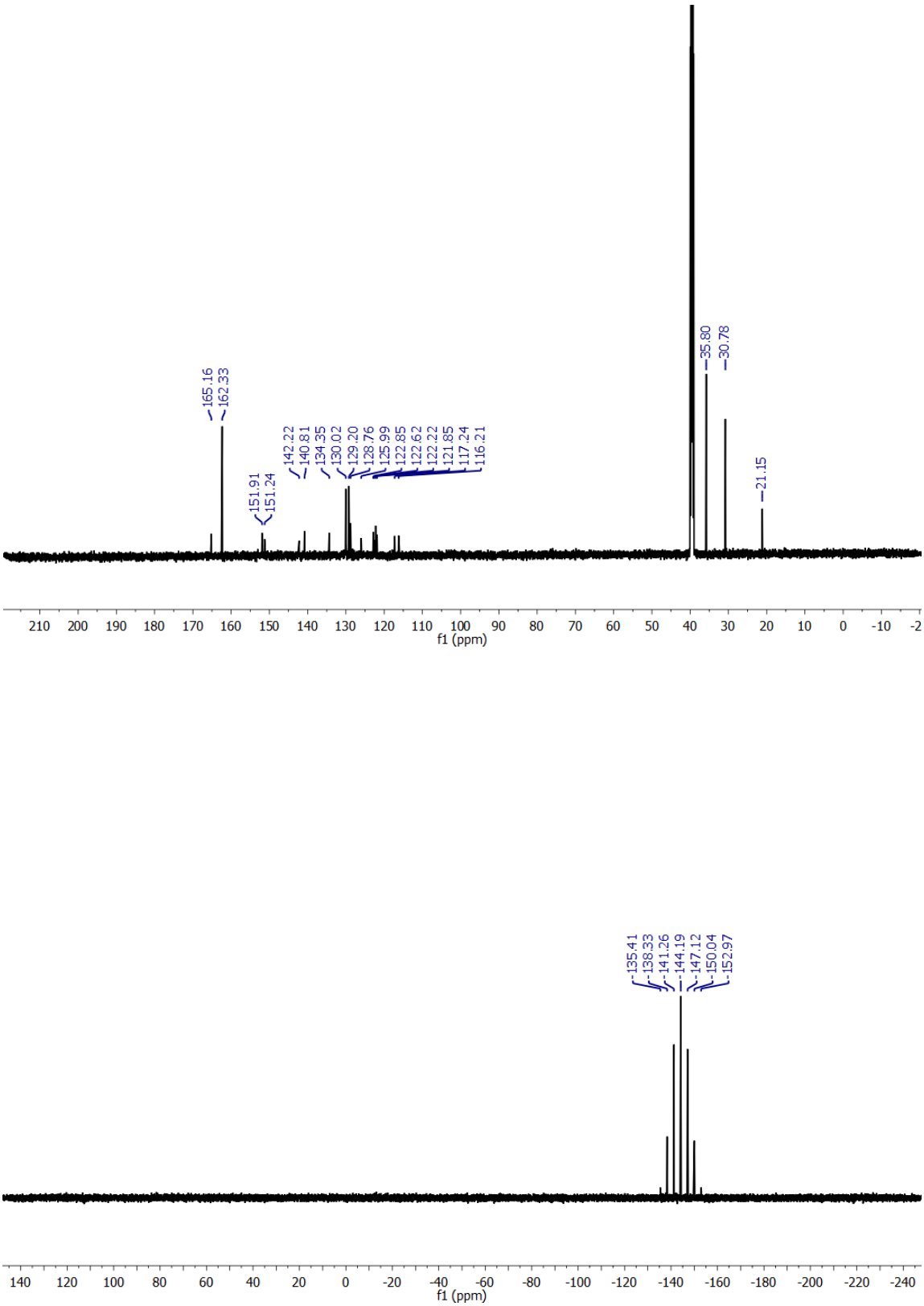
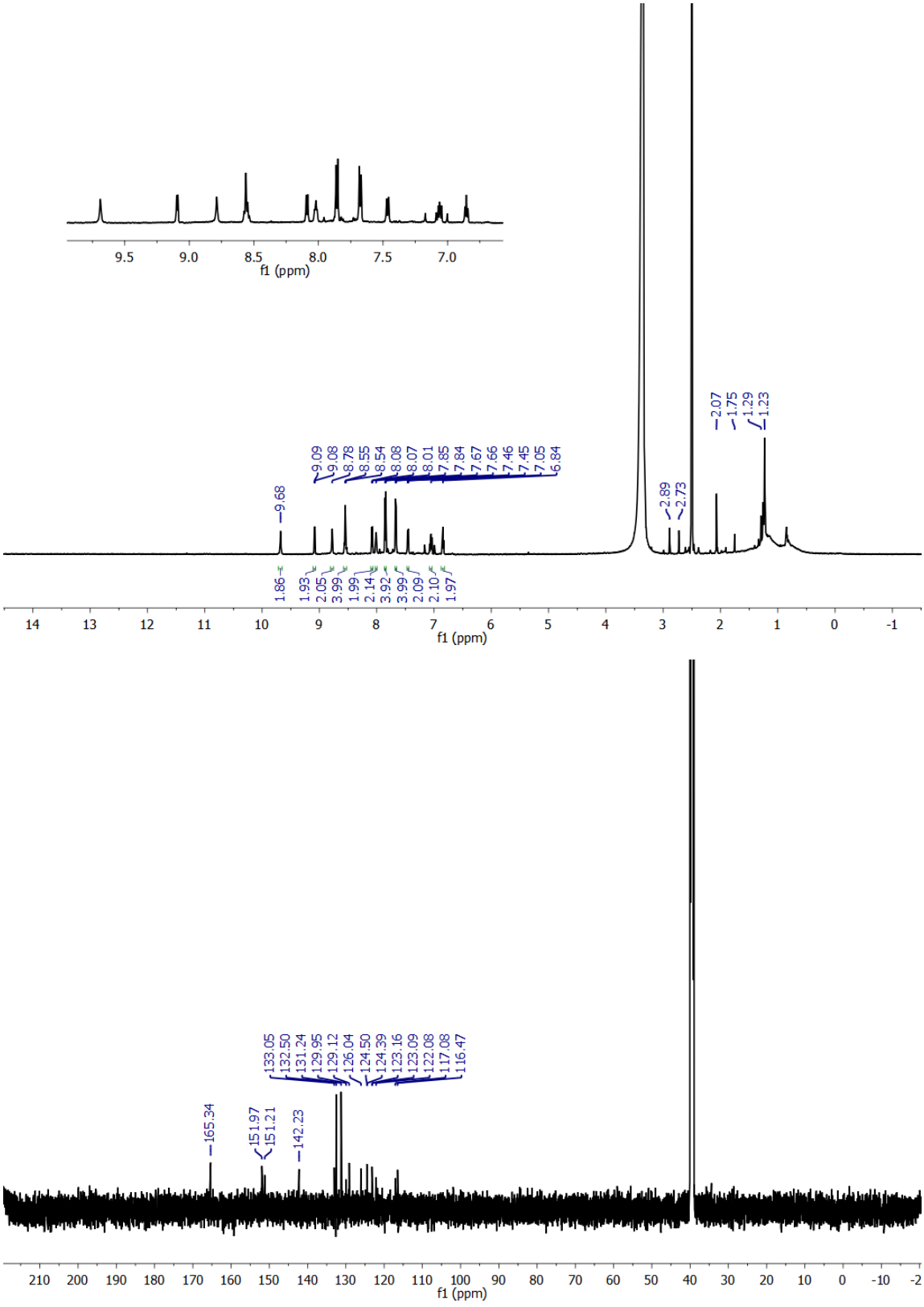


Figure S8. ^{1}H, ^{13}C and ^{31}P NMR spectra of **4**


9.5
9.0
8.5
8.0
7.5
7.0
f1 (ppm)
9.68
9.09
9.08
8.78
8.55
8.54
8.08
8.07
8.01
7.85
7.84
7.67
7.66
7.46
7.45
7.05
6.84
2.89
2.73
2.07
1.75
1.29
1.23
1.86
1.93
2.05
3.99
1.99
2.14
3.92
3.99
2.09
2.10
1.97
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)
165.34
151.97
151.21
142.23
133.05
132.50
131.24
129.95
129.12
126.04
124.50
124.39
123.16
123.09
122.08
117.08
116.47
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-2
f1 (ppm)

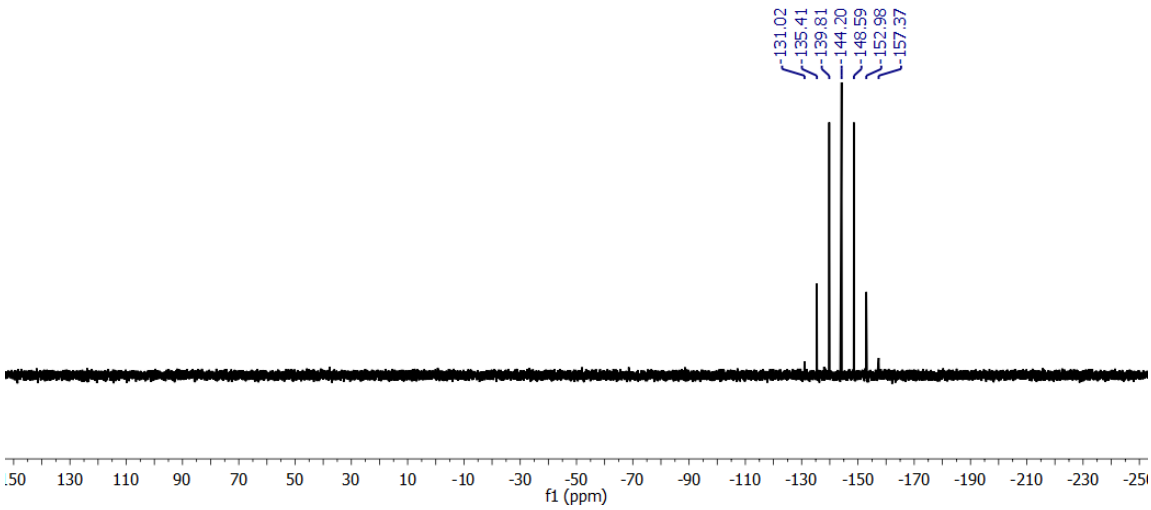
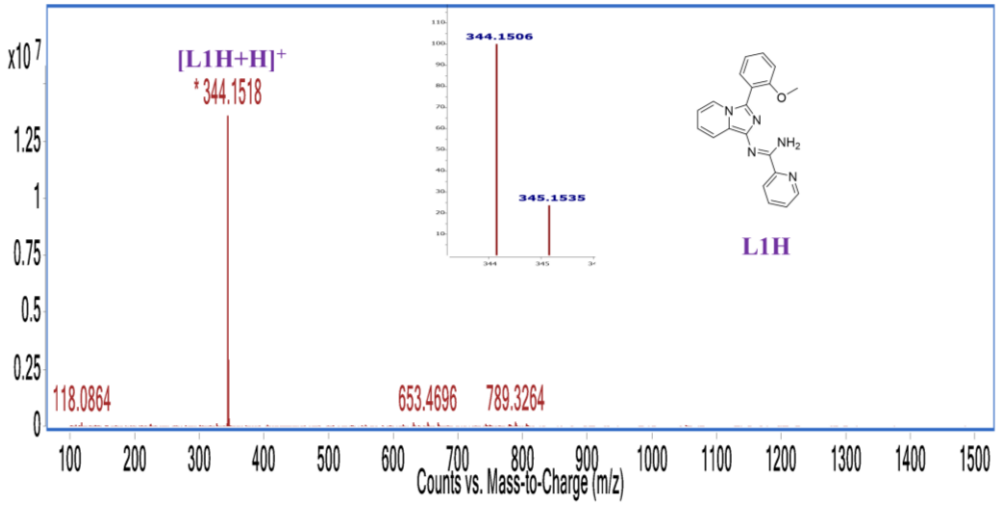


Figure S9. ^{1}H, ^{13}C and ^{31}P NMR spectra of **5**



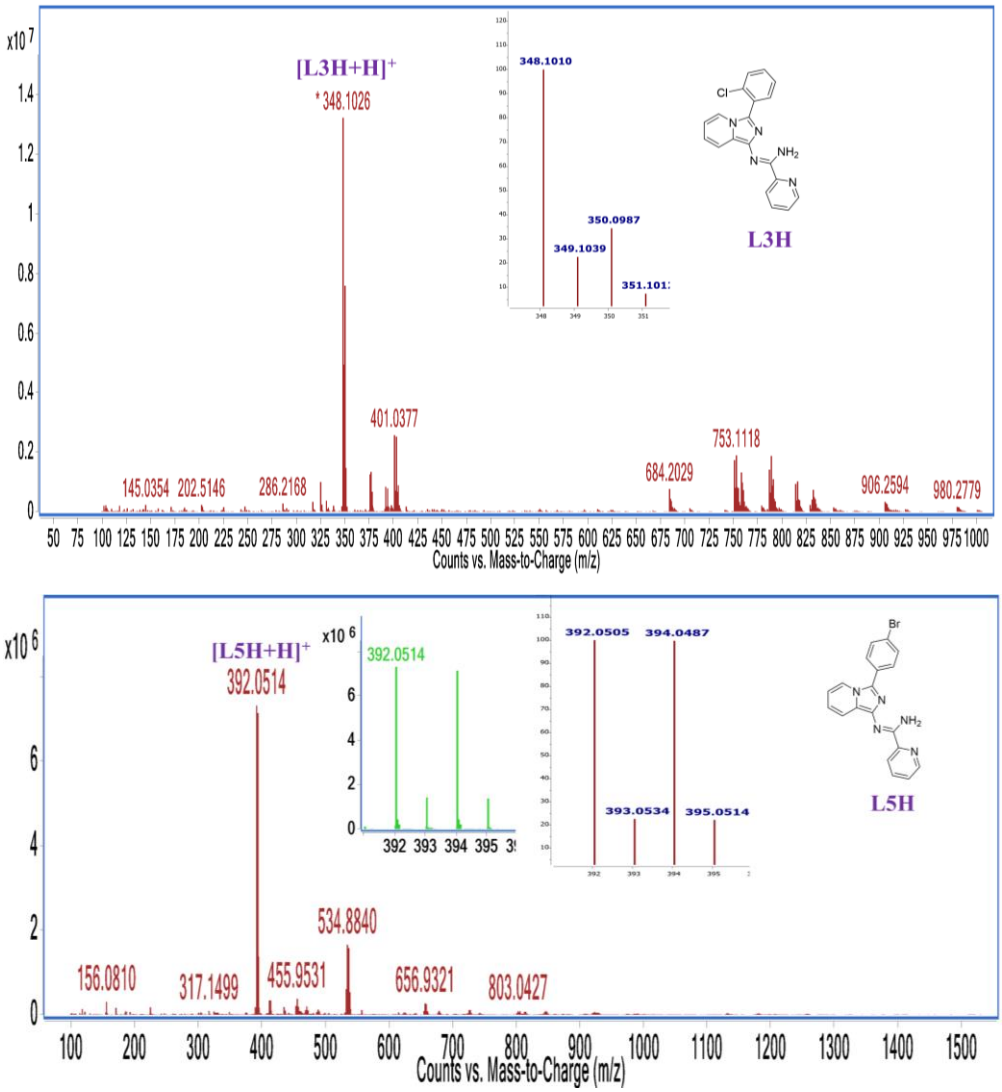


Figure S10. HRMS(ESI) spectrum of **L1H**, **L3H**, and **L5H**

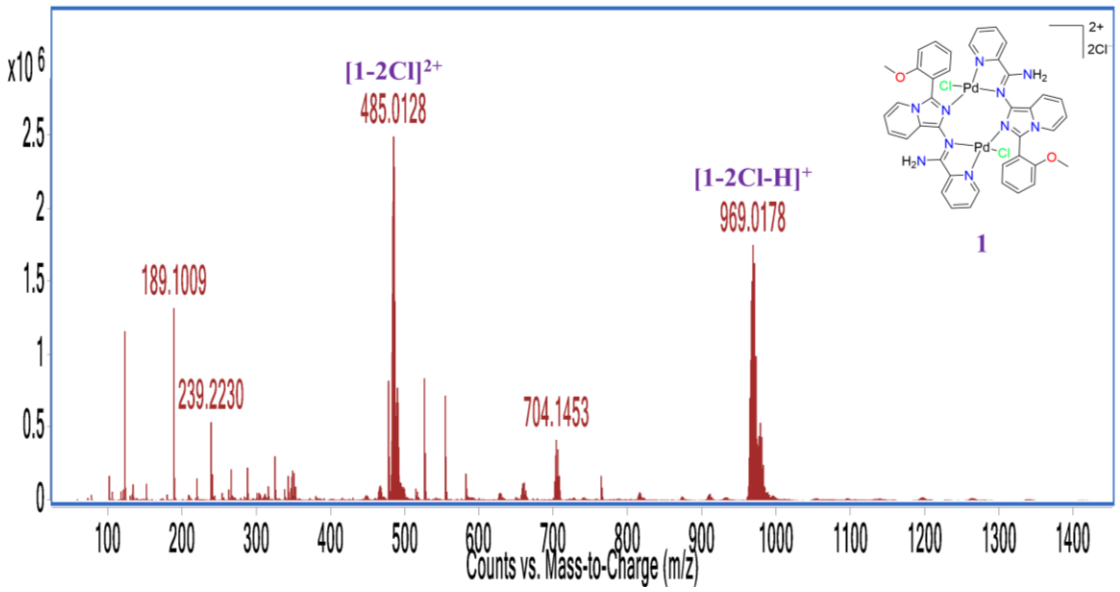


Figure S11A. HRMS(ESI) full spectrum of **1**

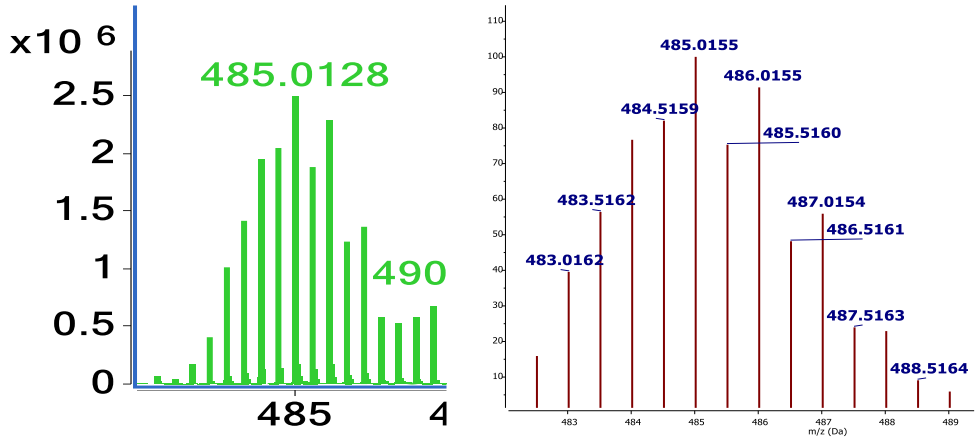


Figure S11B. HRMS(ESI) expanded (left) Simulated (right) spectra of **1** at *m/z* 485.0128

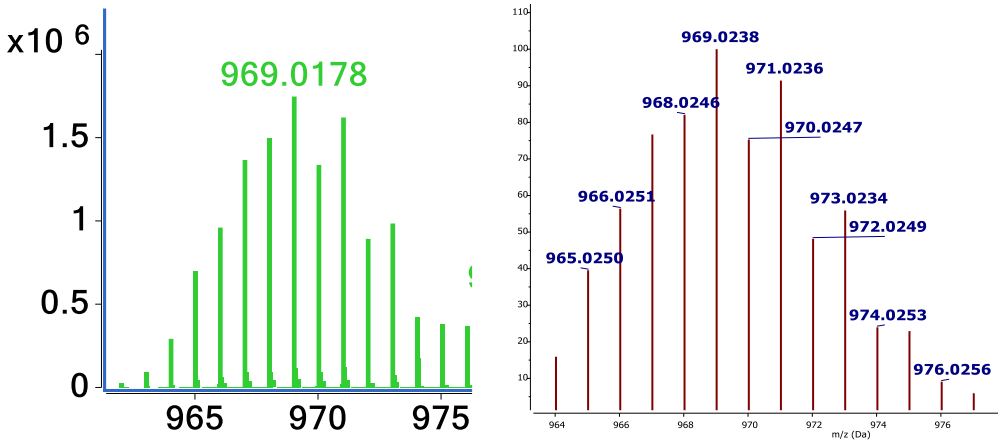


Figure S11C. HRMS(ESI) expanded (left) Simulated (right) spectra of **1** at *m/z* 969.0178

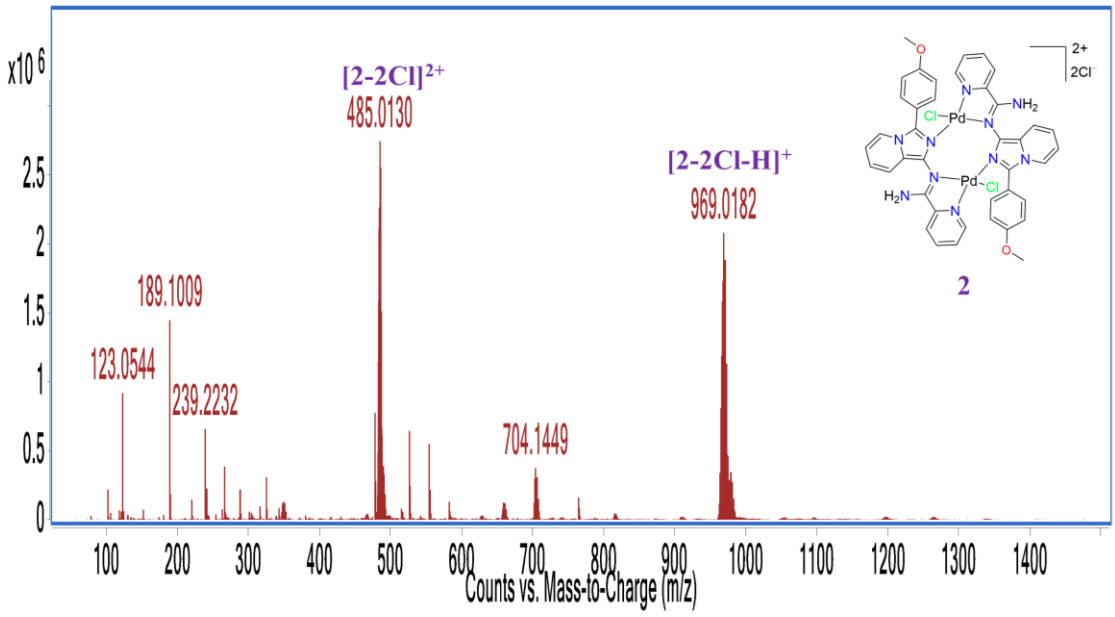


Figure S12A. HRMS(ESI) full spectrum of **2**

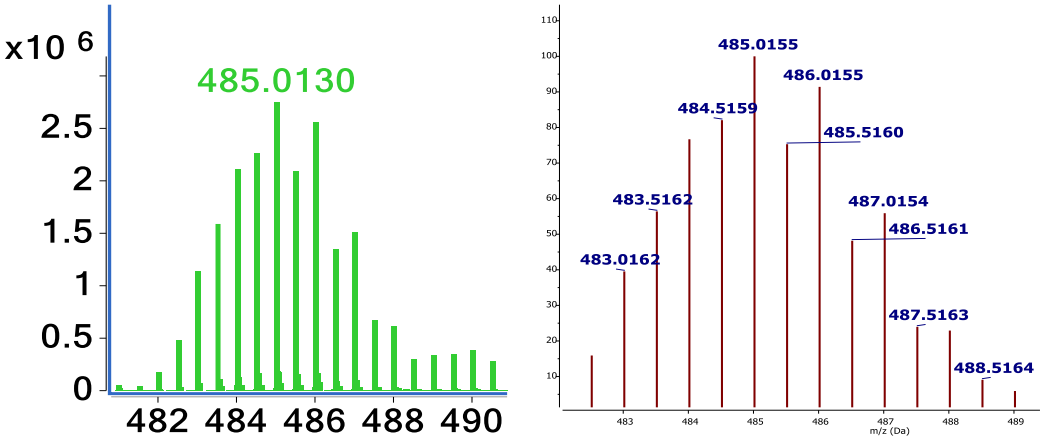


Figure S12B. HRMS(ESI) expanded (left) Simulated (right) spectra of **2** at *m/z* 485.0130

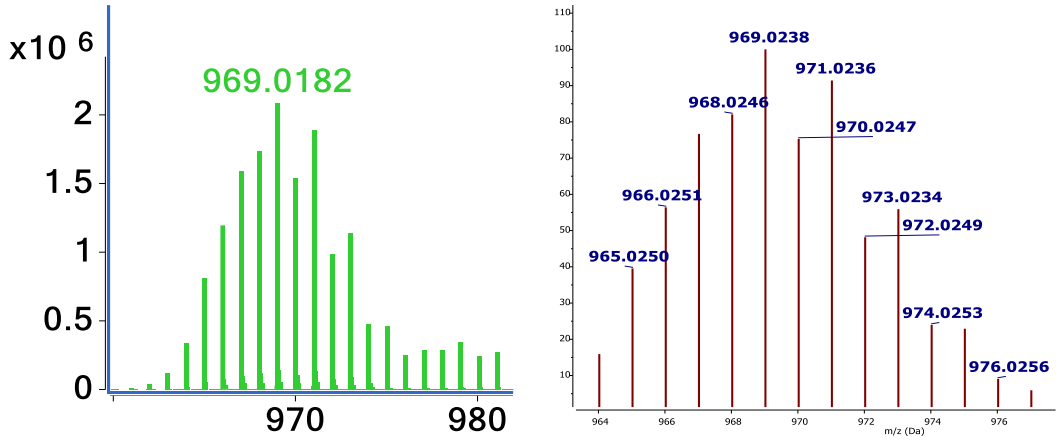


Figure S12C. HRMS(ESI) expanded (left) Simulated (right) spectra of **2** at *m/z* 969.0182

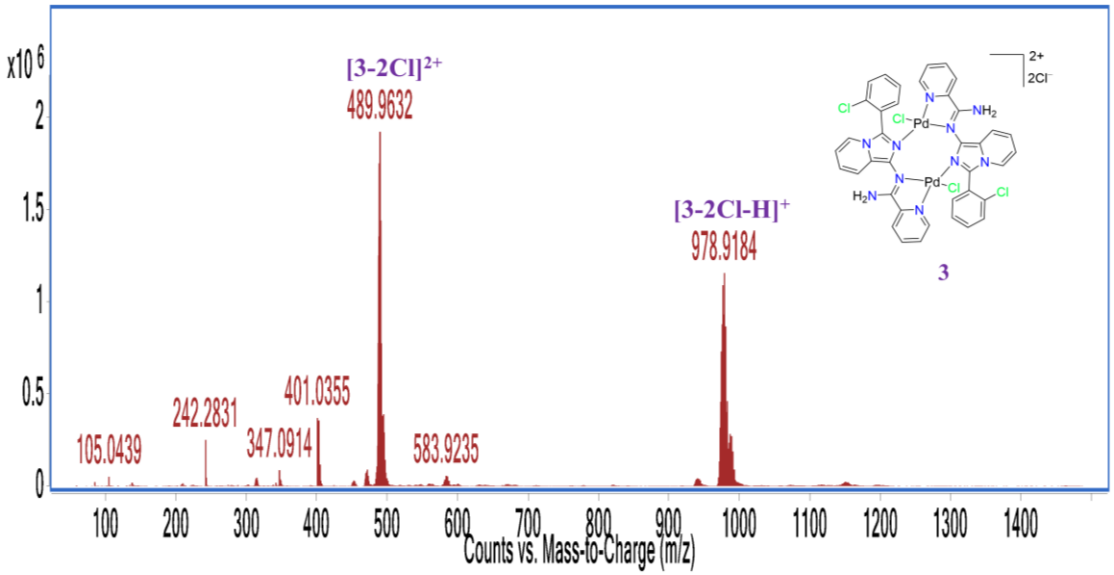


Figure S13A. HRMS(ESI) full spectrum of **3**

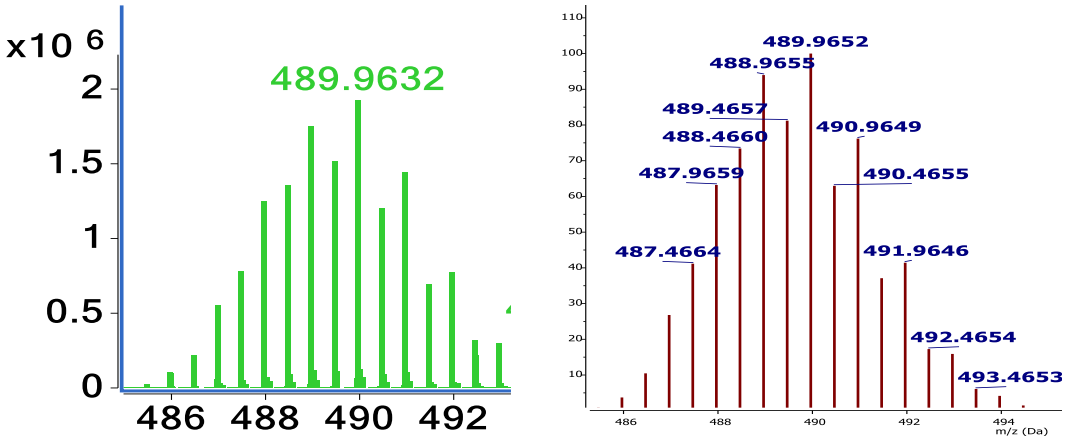


Figure S13B. HRMS(ESI) expanded (left) Simulated (right) spectra of **3** at *m/z* 489.9632

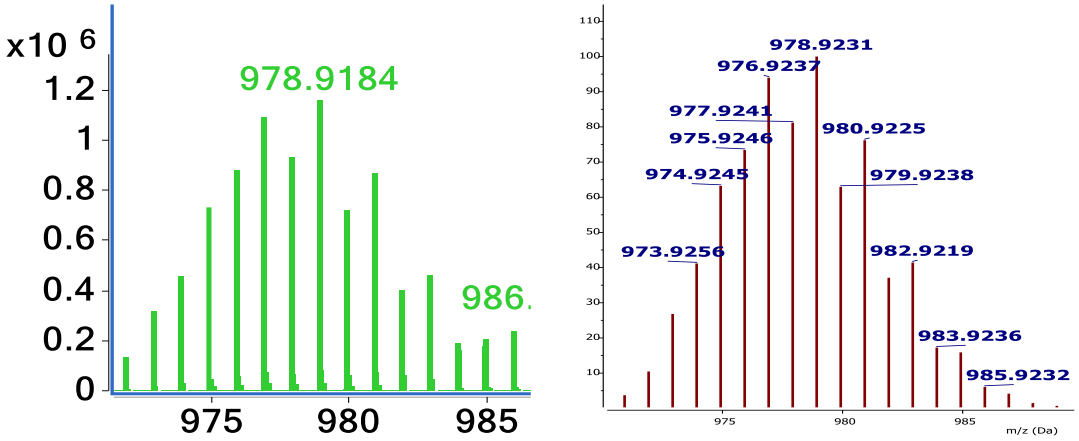


Figure S13C. HRMS(ESI) expanded (left) Simulated (right) spectra of **3** at *m/z* 978.9184

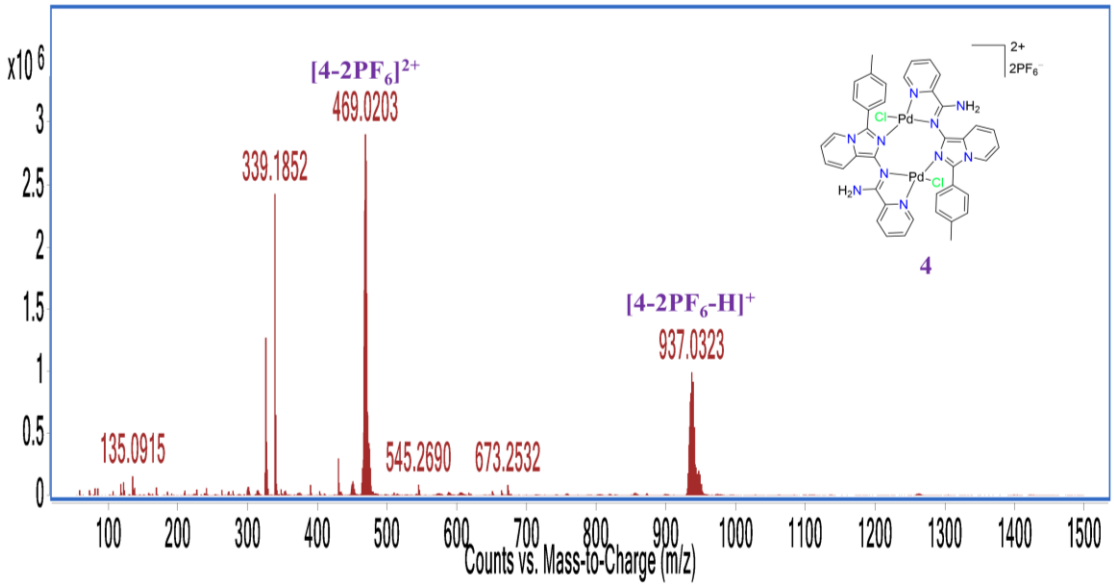


Figure S14A. HRMS(ESI) full spectrum of **4**

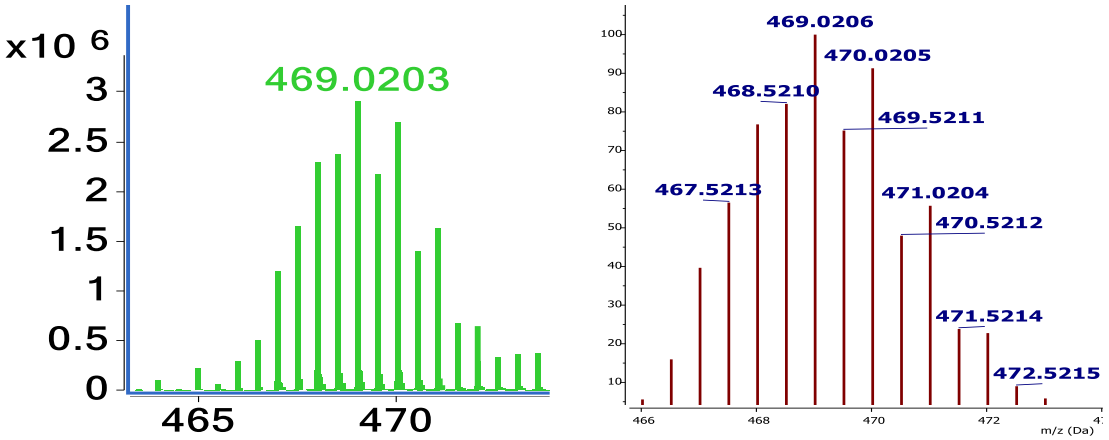


Figure S14B. HRMS(ESI) expanded (left) Simulated (right) spectra of **4** at *m/z* 469.0203

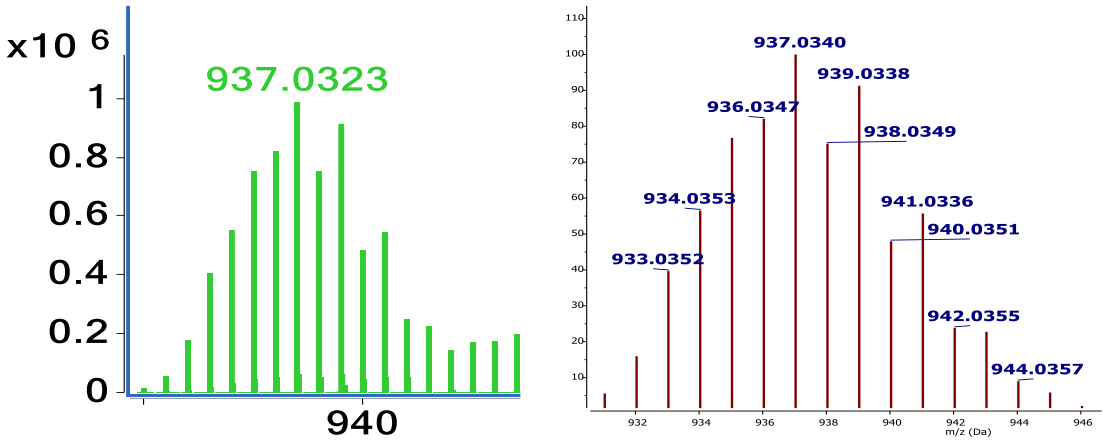


Figure S14C. HRMS(ESI) expanded (left) Simulated (right) spectra of **4** at *m/z* 937.0323

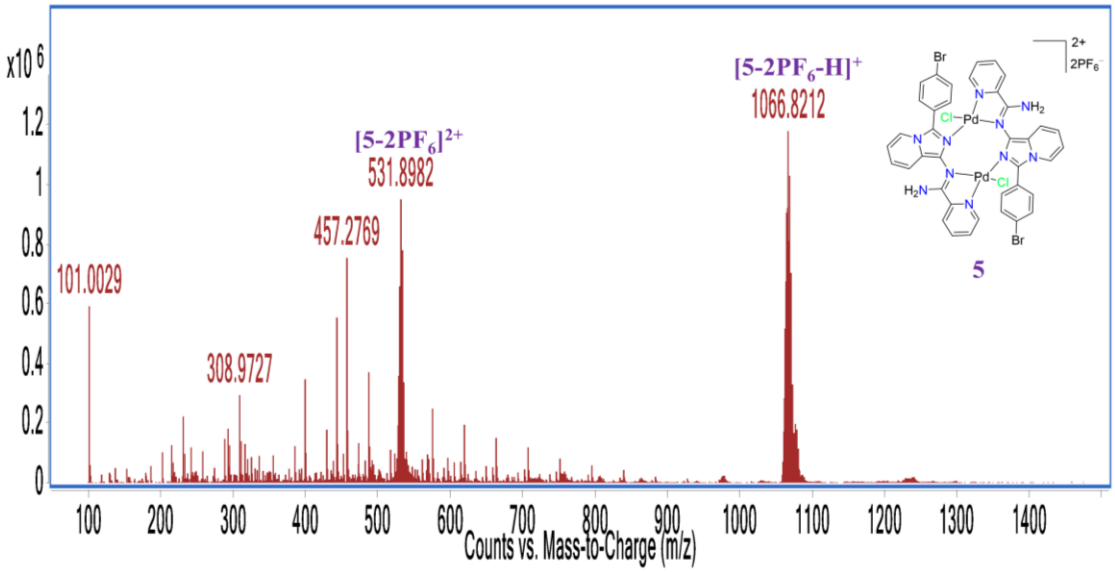


Figure S15A. HRMS(ESI) full spectrum of **5**

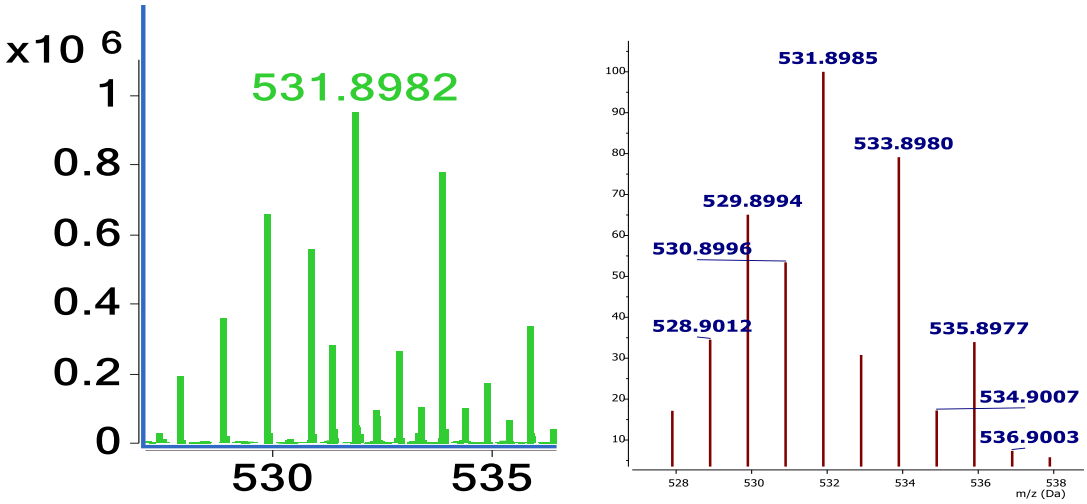


Figure S15B. HRMS(ESI) expanded (left) Simulated (right) spectra of **5** at *m/z* 531.8982

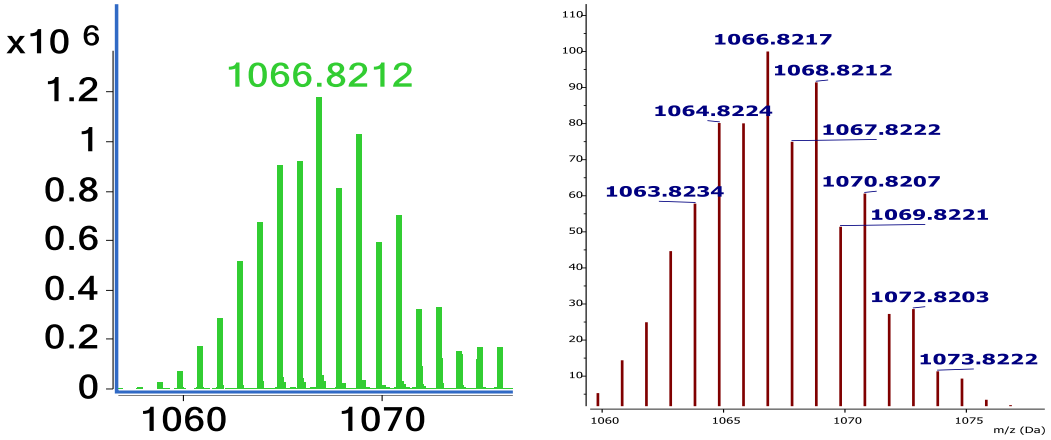
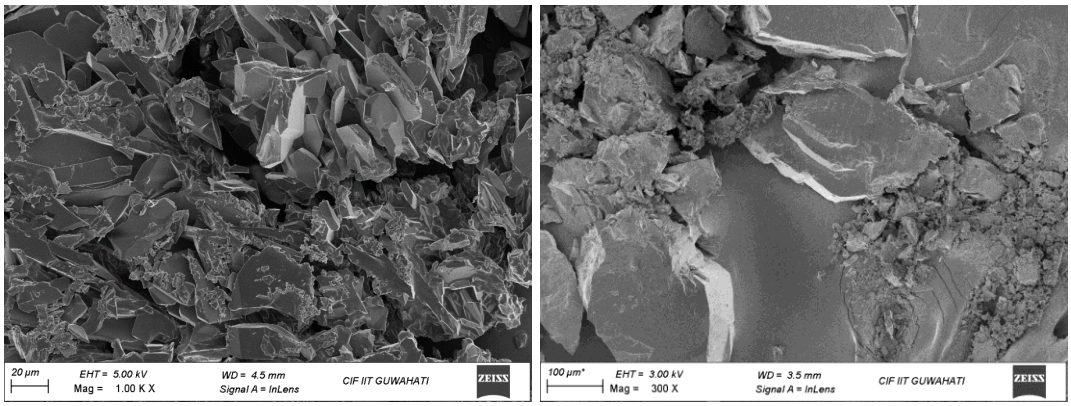
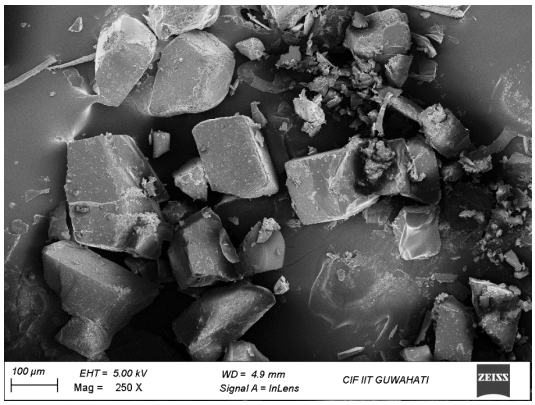


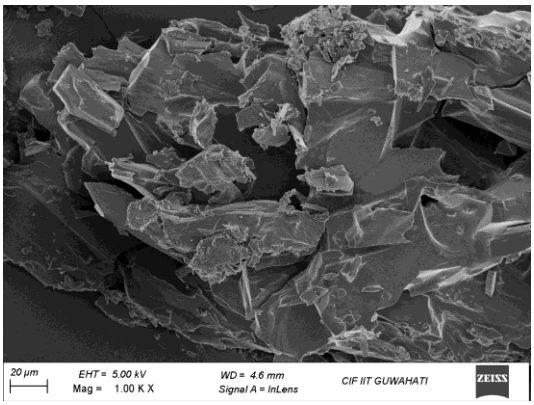
Figure S15C. HRMS(ESI) expanded (left) Simulated (right) spectra of **5** at *m/z* 1066.8212



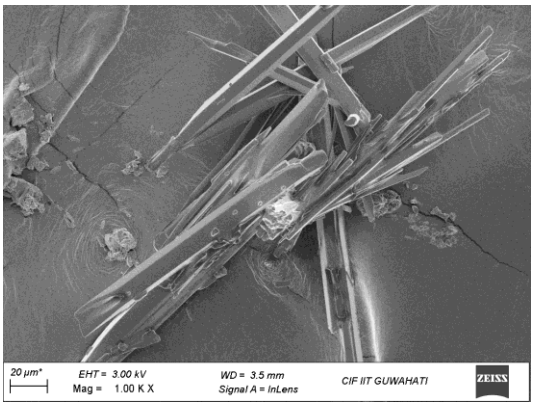
L1H **L2H**



L3H

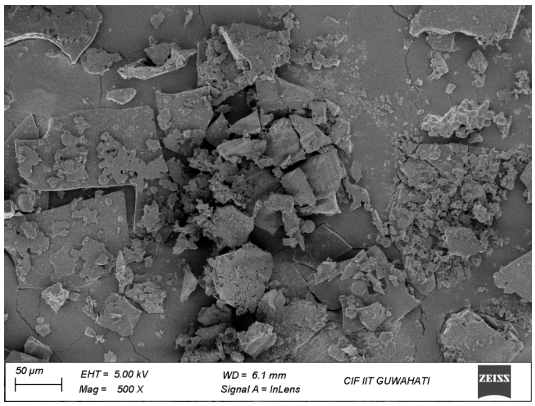


L4H

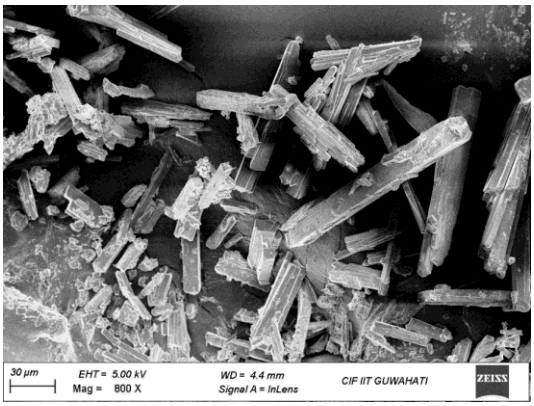


L5H

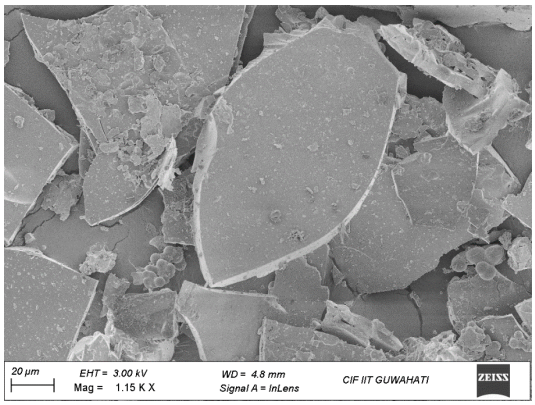
Figure S16. FESEM images of **L1H – L5H**



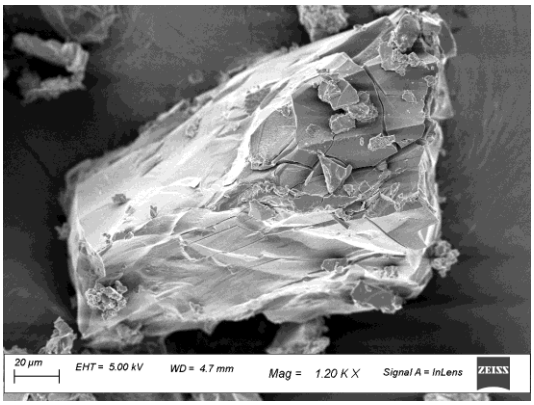
1



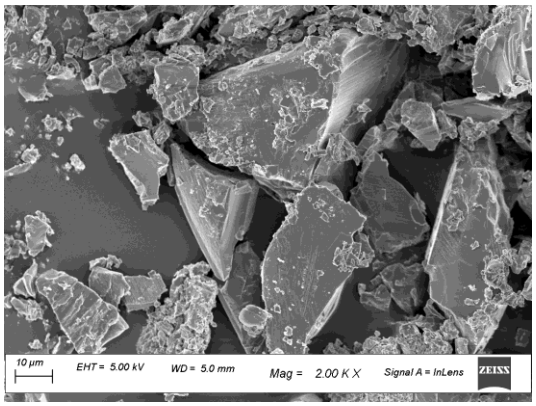
2



3



4



5

Figure S17. FESEM images of **1** – **5**

Crystallographic data

For the single crystal XRD data collection of the appropriate single crystals of **L1H**, **L3H** and **L5H** was mount on a single source Super Nova CCD System instrument from Agilent Technologies equipped with a fine focus 1.75 kW sealed tube with Mo-Kα radiation was used at room temperature. The data were reduced using CrysAlisPro and Autochem2.1 software.[1] For rest of the ligands and complexes, data was collected at room temperature using a Bruker SMART APEX CCD diffractometer equipped with fine focus 1.75 kW sealed tube of Mo-Kα (λ = 0.71073 Å) X-ray source, with increasing ω (width of 0.3° per frame) at a scan speed of either 3 or 5 s per frame.[2] The SMART software was used for data acquisition and the SAINT software for data extraction. The structure solution and refinement were performed on the Olex2-1.5 using the SHELXT, SHELXL programs.[3,4] All atoms except hydrogen atoms are tuned using anisotropic displacement parameters, whereas hydrogen atoms are tuned using relative isotropic parameters.

The disorder in molecular structure of **1g** was fixed using partial occupancies factor, unidentified electron densities were masked using OLEX2 utility.[5] PLATON was used for structure validation and for pictorial visualization of X-ray single crystal data, Mercury and ORTEP software was used.[6–8]

Table S1: Crystallographic data and refinement parameters of **L1H**–**L3H**

Identification code	**L1H**	**L2H**	**L3H**
Empirical formula	$C_{40}H_{34}N_{10}O_2$	$C_{20}H_{17}N_5O$	$C_{19}H_{14}ClN_5$
Formula weight	686.77	343.39	347.80
Temperature/K	297	298.00	293(2)
Crystal system	triclinic	monoclinic	triclinic
Space group	P-1	$P2_1/c$	P-1
a/Å	11.8050(10)	13.5754(9)	8.3384(9)
b/Å	11.9329(10)	10.0125(7)	10.0478(6)
c/Å	13.5763(12)	12.8537(8)	10.3112(7)
α/°	103.728(7)	90	73.262(6)
β/°	91.311(7)	94.760(2)	83.132(7)
γ/°	104.029(8)	90	82.570(7)
Volume/Å^3	1795.8(3)	1741.1(2)	817.26(12)
Z	2	4	2
ρ_{calc}g/cm^3	1.270	1.310	1.413
μ/mm^{-1}	0.083	0.085	0.246
F(000)	720.0	720.0	360.0
Crystal size/mm^3	0.15 × 0.07 × 0.05	0.18 × 0.11 × 0.08	0.17 × 0.08 × 0.07
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.396 to 49.996	5.062 to 54.966	4.946 to 49.998
Index ranges	-14 ≤ h ≤ 12, -14 ≤ k ≤ 14, -16 ≤ l ≤ 16	-17 ≤ h ≤ 17, -12 ≤ k ≤ 12, -16 ≤ l ≤ 16	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -12 ≤ l ≤ 12
Reflections collected	11759	41993	4964
Independent reflections	6303 [R_{int} = 0.0369, R_{sigma} = 0.0960]	3862 [R_{int} = 0.0719, R_{sigma} = 0.0475]	2837 [R_{int} = 0.0388, R_{sigma} = 0.0562]
Data/restraints/parameters	6303/348/472	3862/0/237	2837/0/228
Goodness-of-fit on F^2	1.019	1.169	1.064

Final R indexes [I>=2σ (I)]	R_1 = 0.0745, wR_2 = 0.1679	R_1 = 0.0805, wR_2 = 0.1348	R_1 = 0.0465, wR_2 = 0.1146
Final R indexes [all data]	R_1 = 0.1661, wR_2 = 0.2329	R_1 = 0.1460, wR_2 = 0.1672	R_1 = 0.0676, wR_2 = 0.1347
Largest diff. peak/hole / e Å^{-3}	0.23/-0.18	0.21/-0.18	0.26/-0.23

Table S2: Crystallographic data and refinement parameters of **L4H** and **L5H**

Identification code	**L4H**	**L5H**
Empirical formula	$C_{20}H_{17}N_5$	$C_{19}H_{14}BrN_5$
Formula weight	327.39	392.26
Temperature/K	298.00	293(2)
Crystal system	monoclinic	triclinic
Space group	$P2_1/n$	P-1
a/Å	8.0457(3)	6.7421(5)
b/Å	17.7155(6)	11.0790(13)
c/Å	23.5310(8)	12.2068(15)
α/°	90	75.582(10)
β/°	91.9090(10)	74.358(8)
γ/°	90	87.772(7)
Volume/Å^3	3352.1(2)	849.98(17)
Z	8	2
ρ_{calc}g/cm^3	1.297	1.533
μ/mm^{-1}	0.081	2.430
F(000)	1376.0	396.0
Crystal size/mm^3	0.7 × 0.14 × 0.1	0.14 × 0.08 × 0.04
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.598 to 50.086	4.526 to 50.278
Index ranges	-9 ≤ h ≤ 9, -21 ≤ k ≤ 21, -27 ≤ l ≤ 27	-8 ≤ h ≤ 8, -13 ≤ k ≤ 11, -14 ≤ l ≤ 14
Reflections collected	76157	5226
Independent reflections	5922 [R_{int} = 0.0584, R_{sigma} = 0.0285]	2935 [R_{int} = 0.0739, R_{sigma} = 0.1271]
Data/restraints/parameters	5922/0/453	2935/0/226
Goodness-of-fit on F^2	1.108	0.995
Final R indexes [I>=2σ (I)]	R_1 = 0.0512, wR_2 = 0.1110	R_1 = 0.0732, wR_2 = 0.1652
Final R indexes [all data]	R_1 = 0.0771, wR_2 = 0.1293	R_1 = 0.1261, wR_2 = 0.2051
Largest diff. peak/hole / e Å^{-3}	0.22/-0.21	0.55/-0.84

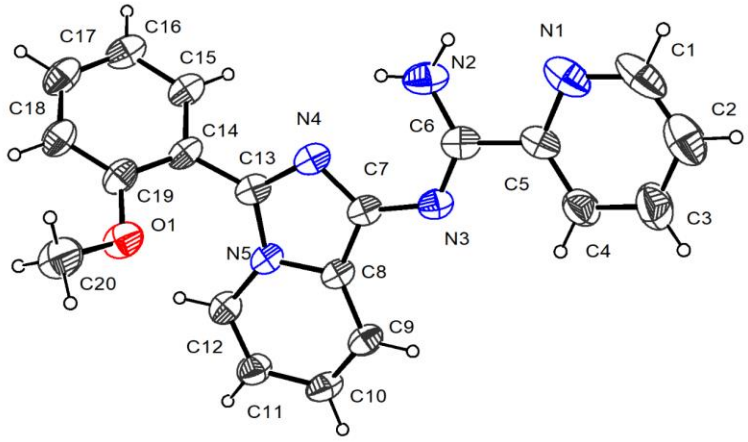


Figure S18. ORTEP diagram of **L1H**. Thermal ellipsoids are drawn at 30% probability level.

Table S3: Bond lengths in **L1H**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C19	1.371(5)	N4	C13	1.337(5)	C8	C9	1.404(6)
O1	C20	1.429(5)	N5	C8	1.403(5)	C9	C10	1.351(6)
N1	C1	1.368(8)	N5	C12	1.394(5)	C10	C11	1.422(6)
N1	C5	1.327(5)	N5	C13	1.380(5)	C11	C12	1.348(6)
N2	C6	1.344(6)	C1	C2	1.362(9)	C13	C14	1.467(6)
N3	C6	1.293(5)	C3	C4	1.377(7)	C14	C15	1.389(6)
N3	C7	1.386(5)	C3	C2	1.352(8)	C14	C19	1.399(6)
N4	C7	1.370(5)	C4	C5	1.386(7)	C15	C16	1.385(6)
C5	C6	1.504(7)	C16	C17	1.391(7)	C18	C19	1.367(7)
C7	C8	1.394(5)	C17	C18	1.362(7)			

Table S4: Bond angels in **L1H**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C19	O1	C20	116.9(4)	C7	C8	N5	105.0(4)
C5	N1	C1	116.0(6)	C7	C8	C9	136.0(5)
C6	N3	C7	121.4(4)	C10	C9	C8	120.0(5)
C13	N4	C7	107.6(4)	C9	C10	C11	119.5(5)
C12	N5	C8	121.4(4)	C12	C11	C10	122.3(5)
C13	N5	C8	107.8(4)	C11	C12	N5	117.8(5)
C13	N5	C12	130.6(4)	N4	C13	N5	109.7(4)
C2	C1	N1	124.0(6)	N4	C13	C14	124.8(4)
C2	C3	C4	119.3(7)	N5	C13	C14	125.5(4)
C3	C4	C5	119.2(5)	C15	C14	C13	118.2(4)

N1	C5	C4	122.8(5)	C15	C14	C19	119.0(5)
N1	C5	C6	115.9(5)	C19	C14	C13	122.5(4)
C4	C5	C6	121.1(4)	C16	C15	C14	120.6(5)
N2	C6	C5	115.6(4)	C15	C16	C17	118.7(5)
N3	C6	N2	127.5(5)	C18	C17	C16	121.0(5)
N3	C6	C5	116.9(5)	C17	C18	C19	120.6(5)
N3	C7	C8	122.3(4)	O1	C19	C14	115.6(5)
N4	C7	N3	127.8(4)	C18	C19	O1	124.3(5)
N4	C7	C8	109.9(4)	C18	C19	C14	120.1(5)
N5	C8	C9	118.9(4)	C3	C2	C1	118.7(7)

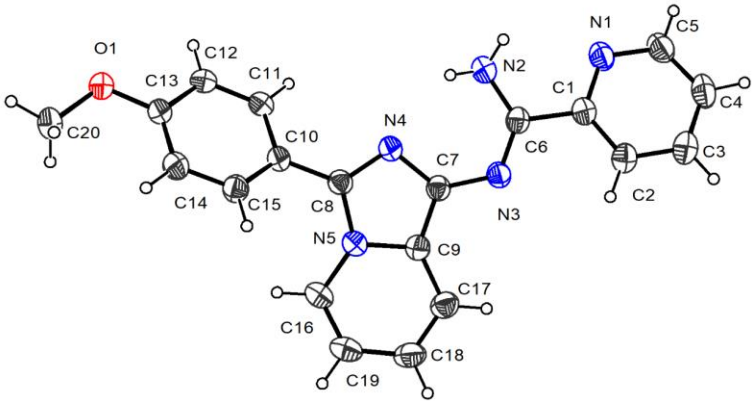


Figure S19. ORTEP diagram of **L2H**. Thermal ellipsoids are drawn at 30% probability level.

Table S5: Bond lengths in **L2H**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C13	1.367(3)	C3	C4	1.372(4)	N5	C16	1.390(3)
O1	C20	1.425(3)	C4	C5	1.370(4)	N2	C6	1.353(3)
N1	C1	1.337(3)	C7	C9	1.388(4)	C1	C2	1.380(4)
N1	C5	1.342(3)	C8	C10	1.456(3)	C1	C6	1.490(4)
N3	C6	1.286(3)	C9	C17	1.405(4)	C2	C3	1.369(4)
N3	C7	1.377(3)	C10	C11	1.394(4)	C14	C15	1.377(4)
N4	C7	1.373(3)	C10	C15	1.388(4)	C16	C19	1.341(4)
N4	C8	1.334(3)	C11	C12	1.372(4)	C17	C18	1.347(4)
N5	C8	1.383(3)	C12	C13	1.387(4)	C18	C19	1.416(4)
N5	C9	1.398(3)	C13	C14	1.375(4)			

Table S6: Bond angels in **L2H**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C13	O1	C20	118.1(2)	N4	C8	N5	110.2(2)

C1	N1	C5	116.6(3)	N4	C8	C10	125.5(2)
C6	N3	C7	122.0(2)	N5	C8	C10	124.1(2)
C8	N4	C7	107.1(2)	N5	C9	C17	119.1(2)
C8	N5	C9	107.2(2)	C7	C9	N5	105.5(2)
C8	N5	C16	132.3(2)	C7	C9	C17	135.4(3)
C16	N5	C9	120.0(2)	C11	C10	C8	120.9(2)
N1	C1	C2	122.6(2)	C15	C10	C8	121.8(2)
N1	C1	C6	116.4(2)	C15	C10	C11	117.2(2)
C2	C1	C6	121.0(3)	C12	C11	C10	121.1(3)
C3	C2	C1	119.7(3)	C11	C12	C13	120.4(3)
C2	C3	C4	118.3(3)	O1	C13	C12	116.5(3)
C5	C4	C3	118.8(3)	O1	C13	C14	124.0(3)
N1	C5	C4	123.9(3)	C14	C13	C12	119.5(3)
N3	C6	N2	127.0(2)	C13	C14	C15	119.6(3)
N3	C6	C1	117.4(2)	C14	C15	C10	122.2(3)
N2	C6	C1	115.6(2)	C19	C16	N5	119.3(3)
N3	C7	C9	121.6(2)	C18	C17	C9	120.2(3)
N4	C7	N3	128.5(2)	C17	C18	C19	119.3(3)
N4	C7	C9	109.9(2)	C16	C19	C18	121.7(3)

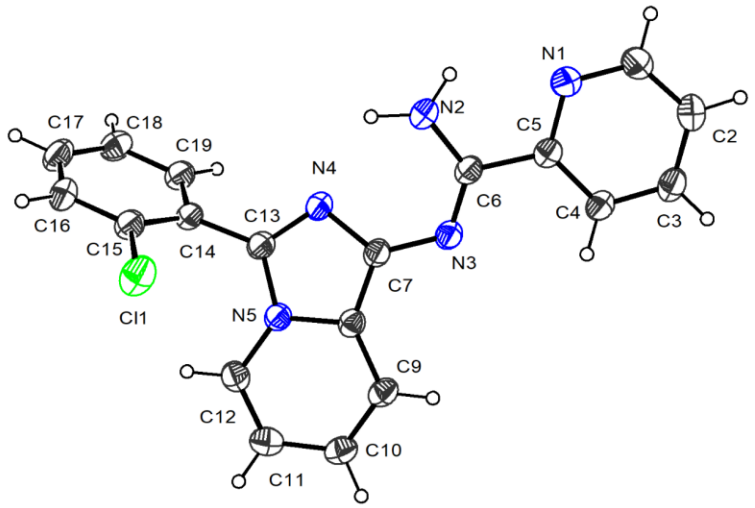


Figure 20. ORTEP diagram of **L3H**. Thermal ellipsoids are drawn at 30% probability level.

Table S7: Bond lengths in **L3H**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C15	1.737(2)	C4	C5	1.379(3)	C13	C14	1.466(3)
N1	C1	1.330(3)	C5	C6	1.477(3)	C14	C15	1.393(3)

N1	C5	1.343(3)	C7	C8	1.390(3)	C14	C19	1.399(3)
N2	C6	1.350(3)	C8	C9	1.409(3)	C15	C16	1.374(3)
N3	C6	1.294(3)	C9	C10	1.351(3)	C16	C17	1.370(3)
N3	C7	1.378(3)	C10	C11	1.409(4)	C17	C18	1.373(3)
N4	C7	1.379(3)	C11	C12	1.346(3)	C18	C19	1.378(3)
C1	C2	1.365(3)	C3	C4	1.368(3)	N5	C13	1.372(3)
C2	C3	1.368(3)	N5	C12	1.383(3)			

Table S8: Bond angels in **L3H**

Atom	Atom	Atom	Atom	Atom	Atom	Angle/°
C1	N1	C5	N5	C8	C9	118.8(2)
C6	N3	C7	C7	C8	C9	135.5(2)
C13	N4	C7	C10	C9	C8	119.5(2)
C12	N5	C8	C9	C10	C11	120.1(2)
C13	N5	C8	C12	C11	C10	121.7(2)
C13	N5	C12	C11	C12	N5	118.3(2)
N1	C1	C2	N4	C13	N5	110.4(2)
C1	C2	C3	N4	C13	C14	124.95(18)
C2	C3	C4	N5	C13	C14	124.6(2)
C3	C4	C5	C15	C14	C13	123.4(2)
N1	C5	C4	C15	C14	C19	117.4(2)
N1	C5	C6	C19	C14	C13	119.1(2)
C4	C5	C6	C14	C15	Cl1	119.75(19)
N2	C6	C5	C16	C15	Cl1	118.31(19)
N3	C6	N2	C16	C15	C14	121.9(2)
N3	C6	C5	C17	C16	C15	119.2(2)
N3	C7	N4	C16	C17	C18	120.7(2)
N3	C7	C8	C17	C18	C19	120.1(2)
N4	C7	C8	C18	C19	C14	120.7(2)
N5	C8	C7				

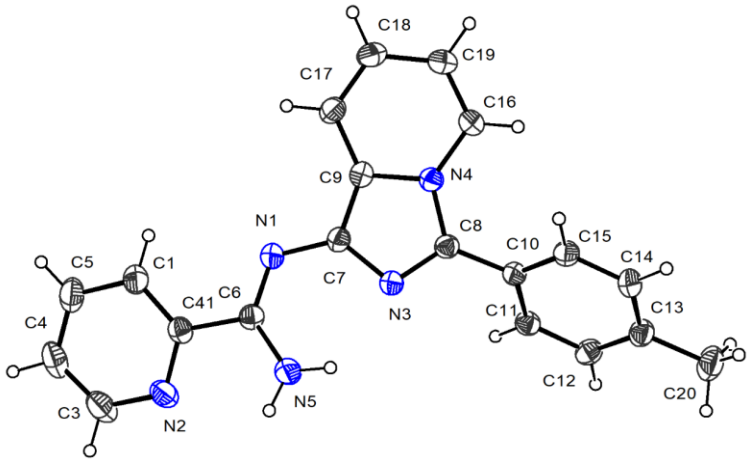


Figure S21. ORTEP diagram of **L4H**. Thermal ellipsoids are drawn at 30% probability level.

Table S9: Bond lengths in **L4H**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C41	1.377(3)	C10	C11	1.394(3)	C10	C11	1.394(3)
C1	C5	1.383(3)	C10	C15	1.390(3)	C10	C15	1.390(3)
N1	C6	1.293(2)	C11	C12	1.377(3)	C11	C12	1.377(3)
N1	C7	1.388(2)	C12	C13	1.386(3)	C12	C13	1.386(3)
N3	C7	1.373(2)	C13	C14	1.381(3)	C13	C14	1.381(3)
N3	C8	1.332(2)	C13	C20	1.506(3)	C13	C20	1.506(3)
N4	C8	1.374(2)	C14	C15	1.378(3)	C14	C15	1.378(3)
N4	C9	1.402(2)	C16	C19	1.339(3)	C16	C19	1.339(3)
N4	C16	1.387(2)	C17	C18	1.353(3)	C17	C18	1.353(3)
N5	C6	1.343(2)	C18	C19	1.418(3)	C18	C19	1.418(3)
N2	C3	1.335(3)	C7	C9	1.383(3)	C4	C5	1.369(3)
C3	C4	1.360(3)	C8	C10	1.459(3)	C9	C17	1.405(3)

Table S10: Bond angels in **L4H**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C41	C1	C5	118.7(2)	C15	C14	C13	121.5(2)
C6	N1	C7	121.32(17)	C14	C15	C10	120.58(19)
C8	N3	C7	107.25(15)	C19	C16	N4	118.93(19)
C8	N4	C9	107.33(15)	C18	C17	C9	120.0(2)
C8	N4	C16	131.42(17)	C17	C18	C19	119.79(19)
C16	N4	C9	121.18(16)	C16	C19	C18	121.5(2)
C1	C41	C6	121.51(19)	C7	C9	N4	105.38(16)
N2	C41	C1	122.69(19)	C7	C9	C17	136.13(19)

N2	C41	C6	115.79(18)	C11	C10	C8	119.03(17)
C41	N2	C3	117.1(2)	C15	C10	C8	122.83(17)
N2	C3	C4	124.0(2)	C15	C10	C11	118.07(18)
C3	C4	C5	118.6(2)	C12	C11	C10	120.63(19)
C4	C5	C1	118.8(2)	C11	C12	C13	121.33(19)
N1	C6	N5	127.33(19)	C12	C13	C20	121.4(2)
N1	C6	C41	117.61(17)	C14	C13	C12	117.84(19)
N5	C6	C41	115.05(18)	C14	C13	C20	120.7(2)
N3	C7	N1	126.69(17)	N3	C8	N4	110.27(16)
N3	C7	C9	109.77(16)	N3	C8	C10	124.61(17)
C9	C7	N1	123.53(17)	N4	C8	C10	125.12(17)
N4	C9	C17	118.48(18)				

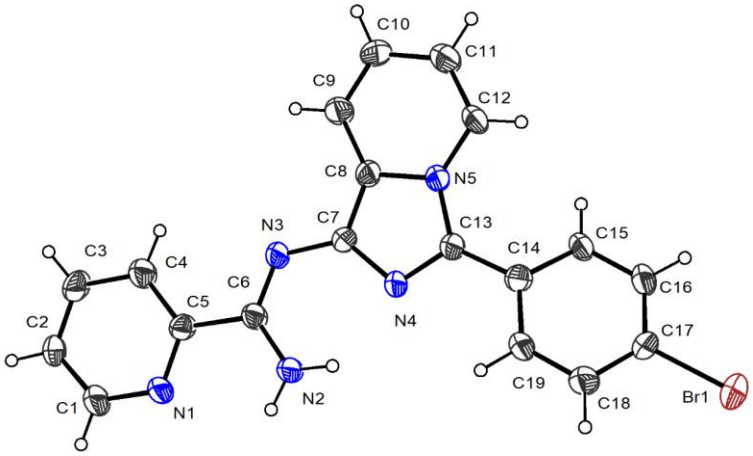


Figure S22. ORTEP diagram of **L5H**. Thermal ellipsoids are drawn at 30% probability level.

Table S11: Bond lengths in **L5H**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C17	1.905(6)	C5	C6	1.493(8)	C9	C10	1.367(8)
N3	C7	1.390(7)	C5	C4	1.388(8)	C2	C3	1.379(9)
N3	C6	1.304(7)	C14	C15	1.411(8)	C2	C1	1.367(9)
N4	C13	1.350(6)	C14	C19	1.398(8)	C8	C7	1.396(7)
N4	C7	1.376(7)	C15	C16	1.390(8)	C8	C9	1.390(8)
N5	C8	1.416(7)	C17	C18	1.381(9)	C13	C14	1.463(8)
N5	C13	1.382(7)	C17	C16	1.366(8)	C4	C3	1.403(9)
N5	C12	1.379(6)	C19	C18	1.373(9)	C12	C11	1.344(9)
N1	C5	1.333(7)	N2	C6	1.336(7)	C10	C11	1.435(9)
N1	C1	1.346(8)						

Table S12: Bond angels in **L5H**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	N3	C7	121.2(5)	N2	C6	C5	117.4(5)
C13	N4	C7	107.2(5)	C15	C14	C13	123.2(5)
C13	N5	C8	107.3(4)	C19	C14	C13	120.0(5)
C12	N5	C8	119.9(5)	C19	C14	C15	116.5(6)
C12	N5	C13	132.6(5)	C16	C15	C14	120.7(5)
C5	N1	C1	117.2(6)	C18	C17	Br1	119.3(5)
C7	C8	N5	105.3(5)	C16	C17	Br1	119.3(5)
C9	C8	N5	120.0(5)	C16	C17	C18	121.4(6)
C9	C8	C7	134.6(6)	C18	C19	C14	122.8(6)
N4	C13	N5	110.2(5)	C10	C9	C8	120.2(6)
N4	C13	C14	121.8(5)	C19	C18	C17	118.5(6)
N5	C13	C14	128.0(5)	C17	C16	C15	119.8(5)
N3	C7	C8	122.6(5)	C1	C2	C3	118.9(6)
N4	C7	N3	127.4(5)	C5	C4	C3	118.3(6)
N4	C7	C8	109.9(5)	C11	C12	N5	119.4(6)
N1	C5	C6	116.6(5)	C2	C3	C4	118.4(6)
N1	C5	C4	123.2(6)	C9	C10	C11	118.3(7)
C4	C5	C6	120.3(5)	N1	C1	C2	123.9(6)
N3	C6	N2	125.4(5)	C12	C11	C10	122.1(6)
N3	C6	C5	117.1(5)				

Table S13: Crystallographic data and refinement parameters of **1**–**3**

Identification code	**1**	**2**	**3**
Empirical formula	$C_{80}H_{68}Cl_4N_{20}O_4Pd_4$ [solvent]	$C_{61}H_{83}Cl_3N_{17}O_9Pd_2$ [solvent]	$C_{38}H_{28}Cl_4N_{10}$ Pd_2 [solvent]
Formula weight	2215.05	1517.59	1162.04
Temperature/K	293.00	298.00	299.00
Crystal system	triclinic	tetragonal	triclinic
Space group	P-1	$I4_1/a$	P-1
a/Å	14.662(2)	29.778(9)	12.611(3)
b/Å	17.696(2)	29.778(9)	13.376(3)
c/Å	19.747(3)	26.221(12)	14.162(3)
α/°	68.860(4)	90	71.220(5)
β/°	78.938(4)	90	80.398(5)
γ/°	88.158(4)	90	78.127(5)
Volume/Å^3	4686.1(11)	23251(18)	2200.3(8)

Z	2	16	2
ρ_{calc}g/cm^3	1.570	1.734	1.754
μ/mm^{-1}	0.938	0.835	1.119
F(000)	2244.0	12528.0	1172.0
Crystal size/mm^3	0.17 × 0.11 × 0.04	? × ? × ?	0.12 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.682 to 50	5.172 to 51.484	3.056 to 57.95
Index ranges	-17 ≤ h ≤ 17, -21 ≤ k ≤ 21, -23 ≤ l ≤ 23	-36 ≤ h ≤ 36, -36 ≤ k ≤ 36, -31 ≤ l ≤ 31	-17 ≤ h ≤ 17, -18 ≤ k ≤ 18, -19 ≤ l ≤ 19
Reflections collected	100506	69701	63247
Independent reflections	16081 [R_{int} = 0.0836, R_{sigma} = 0.0770]	10910 [R_{int} = 0.1156, R_{sigma} = 0.1007]	11528 [R_{int} = 0.0312, R_{sigma} = 0.0253]
Data/restraints/parameters	16081/1688/1016	10910/838/516	11528/2/489
Goodness-of-fit on F^2	1.086	1.045	1.099
Final R indexes [I>=2σ (I)]	R_1 = 0.0897, wR_2 = 0.2205	R_1 = 0.0921, wR_2 = 0.1627	R_1 = 0.0343, wR_2 = 0.0912
Final R indexes [all data]	R_1 = 0.1616, wR_2 = 0.3133	R_1 = 0.1494, wR_2 = 0.1912	R_1 = 0.0439, wR_2 = 0.1016
Largest diff. peak/hole / e Å^{-3}	2.19/-0.92	0.94/-0.62	0.57/-0.79

Table S14: Crystallographic data and refinement parameters of **4** and **5**

Identification code	**4**	**5**
Empirical formula	$C_{49}H_{55}Cl_2F_{12}N_{13}O_3P_2Pd_2$	$C_{41}H_{35}Br_2Cl_2F_{12}N_{11}OP_2Pd_2$
Formula weight	131.65	1577.45
Temperature/K	298.00	297.00
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	11.5271(16)	13.7618(8)
b/Å	16.201(2)	14.2850(8)
c/Å	19.385(3)	14.7187(9)
α/°	74.945(4)	81.543(2)
β/°	75.354(4)	88.825(2)
γ/°	74.117(4)	86.568(2)

Volume/Å^3	3297.5(8)	2856.7(3)
Z	22	2
ρ_{calc}g/cm^3	1.459	1.834
μ/mm^{-1}	0.757	2.271
F(000)	1456.0	1560.0
Crystal size/mm^3	0.19 × 0.15 × 0.12	0.18 × 0.15 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.088 to 54.212	2.888 to 52.732
Index ranges	-14 ≤ h ≤ 14, -20 ≤ k ≤ 20, -24 ≤ l ≤ 24	-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -18 ≤ l ≤ 18
Reflections collected	86769	75307
Independent reflections	14424 [R_{int} = 0.0393, R_{sigma} = 0.0268]	11653 [R_{int} = 0.0549, R_{sigma} = 0.0381]
Data/restraints/parameters	14424/1174/756	11653/1048/660
Goodness-of-fit on F^2	1.032	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0591, wR_2 = 0.1539	R_1 = 0.0561, wR_2 = 0.1415
Final R indexes [all data]	R_1 = 0.0763, wR_2 = 0.1748	R_1 = 0.0934, wR_2 = 0.1768
Largest diff. peak/hole / e Å^{-3}	1.94/-0.83	0.78/-1.29

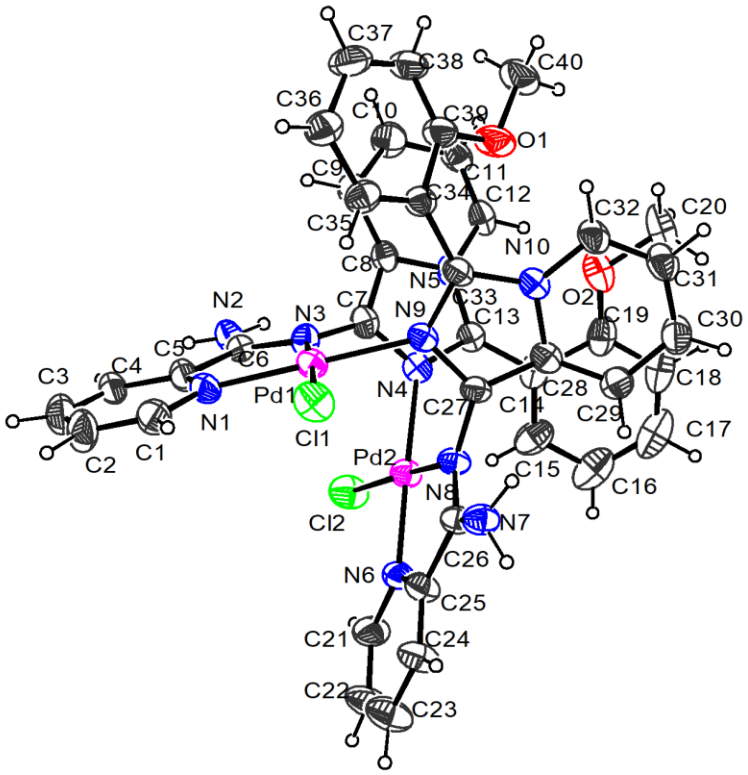


Figure S23. ORTEP diagram of **1**. Thermal ellipsoids are drawn at 30% probability level.

Table S15: Bond lengths in **1**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.293(4)	C27	C28	1.388(18)	N5	C8	1.402(17)
Pd1	N1	1.988(11)	C8	C7	1.395(19)	N5	C13	1.359(16)
Pd1	N9	2.036(10)	C8	C9	1.414(19)	N5	C12	1.381(16)
Pd1	N3	1.992(11)	C33	C34	1.451(18)	N6	C25	1.341(17)
Pd2	Cl2	2.302(4)	C13	C14	1.432(19)	N6	C21	1.333(17)
Pd2	N4	2.062(11)	C34	C35	1.33(2)	N7	C26	1.307(16)
Pd2	N8	1.989(10)	C34	C39	1.45(2)	O1	C39	1.414(19)
Pd2	N6	2.013(11)	C12	C11	1.31(2)	O1	C40	1.407(17)
N4	C13	1.352(16)	C26	C25	1.482(18)	N2	C6	1.326(17)
N4	C7	1.326(17)	C28	C29	1.370(19)	O2	C19	1.36(2)
N8	C27	1.415(15)	C14	C19	1.46(2)	O2	C20	1.418(19)
N8	C26	1.307(16)	C14	C15	1.39(2)	C38	C37	1.38(2)
N10	C33	1.380(16)	C6	C5	1.452(19)	C15	C16	1.35(3)
N10	C28	1.380(16)	C25	C24	1.383(19)	C4	C3	1.35(2)
N10	C32	1.361(16)	C9	C10	1.33(2)	C24	C23	1.38(2)
N1	C5	1.361(18)	C29	C30	1.38(2)	C18	C17	1.34(3)
N1	C1	1.357(18)	C35	C36	1.40(2)	C2	C3	1.39(3)
N9	C27	1.370(16)	C32	C31	1.33(2)	C21	C22	1.40(2)
N9	C33	1.345(15)	C39	C38	1.34(2)	C63	C62	1.33(2)
C11	C10	1.48(2)	C30	C31	1.39(2)	C22	C23	1.32(2)
N3	C6	1.338(16)	C5	C4	1.390(19)	C17	C16	1.38(3)
N3	C7	1.396(17)	C19	C18	1.35(2)	C1	C2	1.36(2)
C56	C55	1.33(2)	C36	C37	1.43(2)			

Table S16: Bond angels in **1**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Pd1	Cl1	95.9(4)	C35	C34	C33	122.5(13)
N1	Pd1	N9	174.9(4)	C35	C34	C39	116.2(14)
N1	Pd1	N3	80.4(5)	C39	C34	C33	121.2(14)
N9	Pd1	Cl1	89.0(3)	N8	C26	N7	124.7(12)
N3	Pd1	Cl1	175.2(3)	N8	C26	C25	114.1(12)
N3	Pd1	N9	94.6(4)	N7	C26	C25	120.8(12)
N4	Pd2	Cl2	89.0(3)	C11	C12	N5	122.3(15)
N8	Pd2	Cl2	176.0(3)	N10	C28	C27	104.7(12)
N8	Pd2	N4	94.2(4)	C29	C28	N10	120.7(12)

N8	Pd2	N6	78.9(4)	C29	C28	C27	134.6(13)
N6	Pd2	Cl2	97.8(3)	N2	C6	N3	122.8(12)
N6	Pd2	N4	172.9(4)	N2	C6	C5	122.6(12)
C13	N4	Pd2	128.9(9)	C13	C14	C19	119.9(15)
C7	N4	Pd2	119.5(9)	C15	C14	C13	121.7(15)
C7	N4	C13	111.5(11)	C15	C14	C19	118.3(15)
C27	N8	Pd2	120.0(8)	N3	C6	C5	114.6(13)
C26	N8	Pd2	117.7(8)	N4	C7	N3	121.1(12)
C26	N8	C27	121.8(11)	N4	C7	C8	108.4(12)
C28	N10	C33	109.4(10)	C8	C7	N3	129.7(13)
C32	N10	C33	129.9(12)	C28	C29	C30	118.8(14)
C32	N10	C28	120.3(12)	C10	C9	C8	117.7(15)
C5	N1	Pd1	115.1(9)	C34	C35	C36	124.9(15)
C1	N1	Pd1	126.6(11)	N6	C25	C26	113.2(12)
C1	N1	C5	118.3(13)	N6	C25	C24	123.2(12)
C6	N3	Pd1	115.7(9)	C24	C25	C26	123.6(13)
C6	N3	C7	121.2(12)	C31	C32	N10	118.6(14)
C7	N3	Pd1	123.0(9)	O1	C39	C34	114.7(13)
C27	N9	Pd1	120.8(8)	C38	C39	O1	122.7(14)
C33	N9	Pd1	131.5(9)	C38	C39	C34	122.6(16)
C33	N9	C27	107.6(11)	C12	C11	C10	118.1(14)
C29	C30	C31	118.0(15)	C25	N6	Pd2	116.0(8)
C13	N5	C8	110.1(11)	C21	N6	Pd2	126.0(11)
C13	N5	C12	130.6(12)	C21	N6	C25	118.1(13)
C12	N5	C8	119.3(12)	C40	O1	C39	116.6(13)
O2	C19	C14	114.5(14)	N1	C5	C6	114.2(12)
C18	C19	O2	126.5(18)	N1	C5	C4	122.0(13)
C18	C19	C14	119.0(19)	C4	C5	C6	123.8(14)
C19	O2	C20	116.2(15)	C32	C31	C30	123.3(15)
N1	C1	C2	119.7(17)	C35	C36	C37	115.7(16)
N9	C27	N8	119.9(11)	C39	C38	C37	118.7(16)
N9	C27	C28	110.1(11)	C16	C15	C14	121(2)
C28	C27	N8	129.8(12)	C3	C4	C5	120.0(17)
C17	C18	C19	119(2)	C23	C24	C25	116.3(16)
N5	C8	C9	120.5(12)	C38	C37	C36	121.7(16)
C7	C8	N5	104.2(12)	C1	C2	C3	122.7(16)
C7	C8	C9	135.2(13)	C9	C10	C11	121.7(16)
N10	C33	C34	127.6(11)	N6	C21	C22	121.5(16)
N9	C33	N10	108.3(11)	C23	C22	C21	118.8(15)

N9	C33	C34	124.1(12)	C4	C3	C2	117.2(16)
N4	C13	N5	105.7(11)	C18	C17	C16	125(2)
N4	C13	C14	126.0(13)	C22	C23	C24	122.1(18)
N5	C13	C14	128.3(12)	C15	C16	C17	118(2)

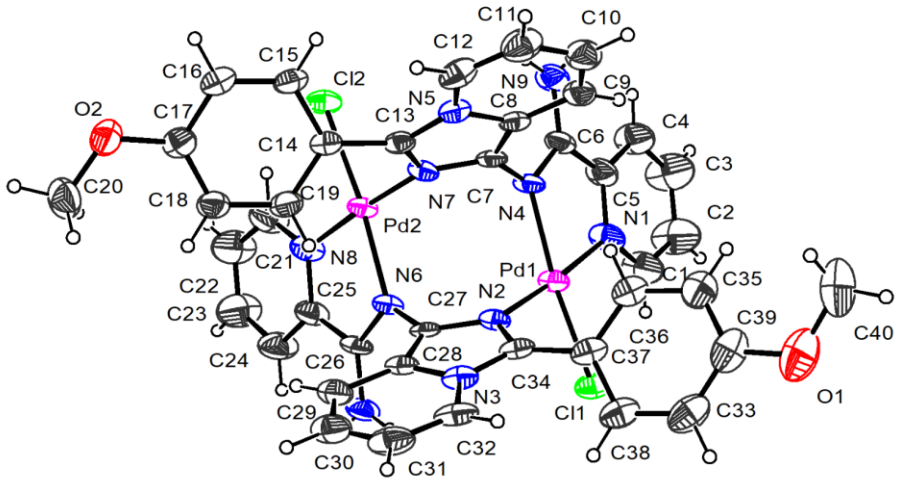


Figure S24. ORTEP diagram of **2**. Thermal ellipsoids are drawn at 30% probability level.

Table S17: Bond lengths in **2**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.300(2)	C5	C6	1.460(12)	C39	C35	1.375(15)
Pd1	N1	2.011(7)	C4	C3	1.380(15)	C35	C36	1.372(13)
Pd1	N2	2.007(6)	C3	C2	1.371(17)	C9	C10	1.350(12)
Pd1	N4	2.036(6)	C2	C1	1.384(15)	C10	C11	1.405(14)
Pd2	Cl2	2.286(2)	C27	C28	1.373(10)	C11	C12	1.330(13)
Pd2	N6	2.016(6)	C28	C29	1.433(12)	C14	C19	1.392(11)
Pd2	N7	2.023(6)	C34	C37	1.449(12)	C14	C15	1.398(11)
Pd2	N8	1.999(7)	C7	C8	1.383(11)	C19	C18	1.390(12)
O1	C39	1.371(13)	C8	C9	1.404(11)	C18	C17	1.382(12)
O1	C40	1.431(17)	C13	C14	1.460(11)	C17	C16	1.376(12)
O2	C20	1.432(12)	C25	C24	1.383(13)	C16	C15	1.366(12)
O2	C17	1.375(10)	C25	C26	1.497(12)	N7	C7	1.366(10)
N1	C5	1.345(11)	C24	C23	1.398(15)	N7	C13	1.329(10)
N1	C1	1.332(12)	C23	C22	1.349(16)	N8	C25	1.345(11)
N2	C27	1.380(10)	C22	C21	1.385(15)	N8	C21	1.322(12)
N2	C34	1.334(10)	C29	C30	1.344(13)	N9	C6	1.316(10)
N3	C28	1.383(10)	C30	C31	1.383(15)	N10	C26	1.303(10)
N3	C34	1.379(10)	C31	C32	1.341(14)	C5	C4	1.373(12)

N3	C32	1.375(10)	C37	C38	1.383(12)	N5	C13	1.376(10)
N4	C6	1.312(10)	C37	C36	1.383(12)	N5	C12	1.382(11)
N4	C7	1.406(10)	C38	C33	1.361(14)	N6	C27	1.408(10)
N5	C8	1.404(10)	C33	C39	1.396(16)	N6	C26	1.303(10)

Table S18: Bond angels in **2**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Pd1	Cl1	96.0(2)	N2	C34	C37	126.6(8)
N1	Pd1	N4	80.1(3)	N3	C34	C37	124.8(8)
N2	Pd1	Cl1	88.15(18)	N4	C6	N9	123.8(8)
N2	Pd1	N1	175.8(3)	N4	C6	C5	116.3(8)
N2	Pd1	N4	95.8(3)	N9	C6	C5	119.8(8)
N4	Pd1	Cl1	173.9(2)	N7	C7	N4	122.0(7)
N6	Pd2	Cl2	174.4(2)	N7	C7	C8	109.7(7)
N6	Pd2	N7	96.4(3)	C8	C7	N4	128.3(8)
N7	Pd2	Cl2	87.63(19)	N5	C8	C9	119.4(8)
N8	Pd2	Cl2	96.0(2)	C7	C8	N5	104.7(8)
N8	Pd2	N6	79.9(3)	C7	C8	C9	135.9(9)
N8	Pd2	N7	176.3(3)	N5	C13	C14	126.3(8)
C39	O1	C40	117.0(12)	N7	C13	N5	108.9(7)
C17	O2	C20	118.3(8)	N7	C13	C14	124.7(8)
C5	N1	Pd1	114.7(6)	N8	C25	C24	122.6(10)
C1	N1	Pd1	126.0(7)	N8	C25	C26	113.5(8)
C1	N1	C5	119.3(9)	C24	C25	C26	123.8(9)
C27	N2	Pd1	126.6(5)	C25	C24	C23	117.5(10)
C34	N2	Pd1	124.9(6)	C22	C23	C24	120.5(12)
C34	N2	C27	108.1(7)	C23	C22	C21	117.7(12)
C34	N3	C28	108.3(7)	N8	C21	C22	124.1(11)
C32	N3	C28	121.9(8)	C30	C29	C28	117.3(10)
C32	N3	C34	129.9(9)	C29	C30	C31	122.0(11)
C6	N4	Pd1	114.2(6)	C32	C31	C30	121.8(10)
C6	N4	C7	120.4(7)	C31	C32	N3	118.1(10)
C7	N4	Pd1	124.3(5)	C38	C37	C34	121.7(9)
C13	N5	C8	108.2(7)	C38	C37	C36	118.2(10)
C13	N5	C12	131.0(8)	C36	C37	C34	120.1(8)
C12	N5	C8	120.8(8)	C33	C38	C37	120.3(11)
C27	N6	Pd2	122.3(5)	C38	C33	C39	120.7(11)
C26	N6	Pd2	116.1(6)	O1	C39	C33	116.6(12)
C26	N6	C27	119.8(7)	O1	C39	C35	123.9(13)

C7	N7	Pd2	127.7(5)	C35	C39	C33	119.5(11)
C13	N7	Pd2	123.1(6)	C36	C35	C39	118.9(11)
C13	N7	C7	108.4(7)	C35	C36	C37	122.2(10)
C25	N8	Pd2	115.7(6)	C10	C9	C8	118.5(9)
C21	N8	Pd2	126.7(7)	C9	C10	C11	120.7(10)
C21	N8	C25	117.5(9)	C12	C11	C10	122.1(10)
N1	C5	C4	120.9(9)	C11	C12	N5	118.5(10)
N1	C5	C6	114.5(8)	C19	C14	C13	120.7(8)
C4	C5	C6	124.5(9)	C19	C14	C15	117.5(8)
C5	C4	C3	118.5(11)	C15	C14	C13	121.5(8)
C2	C3	C4	121.7(12)	C18	C19	C14	122.1(8)
C3	C2	C1	115.9(12)	C17	C18	C19	118.5(9)
N1	C1	C2	123.6(11)	O2	C17	C18	122.8(9)
N2	C27	N6	122.6(7)	O2	C17	C16	117.1(8)
C28	C27	N2	108.8(7)	C16	C17	C18	120.1(9)
C28	C27	N6	128.5(8)	C15	C16	C17	121.3(9)
N3	C28	C29	118.9(8)	C16	C15	C14	120.5(9)
C27	C28	N3	106.1(8)	N6	C26	N10	125.4(9)
C27	C28	C29	135.0(9)	N6	C26	C25	114.6(7)
N2	C34	N3	108.6(8)	N10	C26	C25	119.9(8)

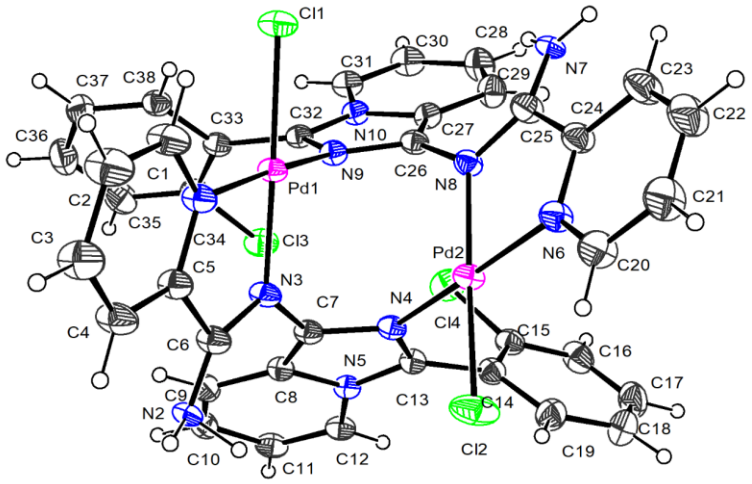


Figure S25. ORTEP diagram of **3**. Thermal ellipsoids are drawn at 30% probability level.

Table S19: Bond lengths in **3**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.3105(8)	C33	C34	1.396(4)	C31	C30	1.345(5)

Pd1	N9	2.033(2)	C8	C9	1.412(4)	C34	C35	1.385(5)
Pd1	N3	1.991(2)	C25	C29	1.417(4)	C10	C11	1.419(5)
Pd1	N1	2.013(2)	C6	C5	1.502(4)	C20	C21	1.377(5)
Pd2	Cl2	2.3158(10)	C6	N2	1.249(6)	C37	C36	1.384(6)
Pd2	N4	2.030(2)	N8	C26	1.342(4)	C1	C2	1.381(5)
Pd2	N8	2.016(2)	C24	C26	1.506(5)	C29	C28	1.347(5)
Pd2	N6	2.016(3)	C24	C23	1.373(5)	C16	C17	1.369(6)
Cl3	C34	1.739(3)	C14	C15	1.395(4)	C4	C3	1.384(5)
Cl4	C15	1.734(3)	C14	C19	1.397(5)	C2	C3	1.375(6)
N9	C32	1.338(3)	C38	C37	1.368(5)	C19	C18	1.386(5)
N9	C27	1.366(4)	C9	C10	1.355(4)	C23	C22	1.378(6)
N4	C7	1.370(4)	C5	C4	1.375(4)	C35	C36	1.379(6)
N4	C13	1.338(3)	C26	N7	1.260(6)	C28	C30	1.415(5)
N3	C7	1.389(3)	N8	C27	1.387(4)	C18	C17	1.374(6)
N3	C6	1.347(4)	C15	C16	1.382(5)	C21	C22	1.363(6)
N10	C32	1.363(3)	C12	C11	1.344(4)	C32	C33	1.464(4)
N10	C25	1.397(4)	N1	C5	1.343(4)	C7	C8	1.376(4)
N10	C31	1.393(3)	N1	C1	1.335(4)	C27	C25	1.382(4)
N5	C13	1.363(4)	N6	C24	1.342(4)	C13	C14	1.473(4)
N5	C8	1.396(3)	N6	C20	1.342(4)	C33	C38	1.408(4)
N5	C12	1.390(3)						

Table S20: Bond angels in **3**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N9	Pd1	Cl1	89.78(7)	C7	C8	C9	135.8(3)
N3	Pd1	Cl1	175.59(7)	N10	C25	C29	118.5(3)
N3	Pd1	N9	94.54(9)	C27	C25	N10	105.4(2)
N3	Pd1	N1	80.75(10)	C27	C25	C29	136.0(3)
N1	Pd1	Cl1	94.99(7)	N3	C6	C5	111.6(3)
N1	Pd1	N9	174.07(10)	N2	C6	N3	125.9(5)
N4	Pd2	Cl2	88.69(7)	N2	C6	C5	121.8(5)
N8	Pd2	Cl2	175.55(7)	N5	C8	C9	118.6(3)
N8	Pd2	N4	95.62(9)	C7	C8	N5	105.6(2)
N8	Pd2	N6	80.40(10)	N6	C24	C26	116.1(3)
N6	Pd2	Cl2	95.36(8)	N6	C24	C23	121.7(3)
N6	Pd2	N4	174.84(10)	C23	C24	C26	122.1(3)
C32	N9	Pd1	125.74(19)	C15	C14	C13	122.1(3)
C32	N9	C27	109.3(2)	C15	C14	C19	117.5(3)
C27	N9	Pd1	123.86(18)	C19	C14	C13	120.3(3)

C7	N4	Pd2	123.85(18)	C37	C38	C33	121.0(3)
C13	N4	Pd2	127.5(2)	C10	C9	C8	119.9(3)
C13	N4	C7	108.6(2)	N1	C5	C6	116.3(3)
C7	N3	Pd1	121.41(18)	N1	C5	C4	121.4(3)
C6	N3	Pd1	117.10(19)	C4	C5	C6	122.3(3)
C6	N3	C7	121.5(2)	N8	C26	C24	112.1(3)
C32	N10	C25	108.8(2)	N7	C26	N8	125.8(5)
C32	N10	C31	129.3(3)	N7	C26	C24	121.0(5)
C31	N10	C25	121.6(2)	C16	C17	C18	120.5(4)
C13	N5	C8	108.5(2)	C21	C22	C23	119.4(4)
C13	N5	C12	130.2(2)	C14	C15	Cl4	120.2(2)
C12	N5	C8	121.1(2)	C16	C15	Cl4	118.3(3)
C27	N8	Pd2	123.69(19)	C16	C15	C14	121.5(3)
C26	N8	Pd2	116.3(2)	C11	C12	N5	118.8(3)
C26	N8	C27	120.0(3)	C30	C31	N10	118.4(3)
C5	N1	Pd1	113.81(19)	C33	C34	Cl3	120.1(2)
C1	N1	Pd1	126.4(2)	C35	C34	Cl3	118.2(3)
C1	N1	C5	119.8(3)	C35	C34	C33	121.7(3)
C24	N6	Pd2	114.0(2)	C9	C10	C11	119.6(3)
C20	N6	Pd2	126.7(2)	C12	C11	C10	121.7(3)
C20	N6	C24	119.3(3)	N6	C20	C21	121.1(4)
N9	C32	N10	108.0(2)	C38	C37	C36	120.4(3)
N9	C32	C33	126.9(2)	N1	C1	C2	121.2(3)
N10	C32	C33	125.0(2)	C28	C29	C25	119.2(3)
N4	C7	N3	120.9(2)	C17	C16	C15	119.5(4)
N4	C7	C8	108.8(2)	C5	C4	C3	119.3(3)
C8	C7	N3	130.1(3)	C3	C2	C1	119.6(3)
N9	C27	N8	119.9(2)	C18	C19	C14	120.7(4)
N9	C27	C25	108.4(3)	C24	C23	C22	118.9(4)
C25	C27	N8	131.7(3)	C2	C3	C4	118.7(3)
N4	C13	N5	108.5(2)	C36	C35	C34	119.3(3)
N4	C13	C14	127.6(3)	C29	C28	C30	120.9(3)
N5	C13	C14	123.8(2)	C17	C18	C19	120.1(4)
C38	C33	C32	120.5(3)	C22	C21	C20	119.6(4)
C34	C33	C32	122.3(3)	C31	C30	C28	121.3(3)
C34	C33	C38	117.2(3)	C35	C36	C37	120.2(3)

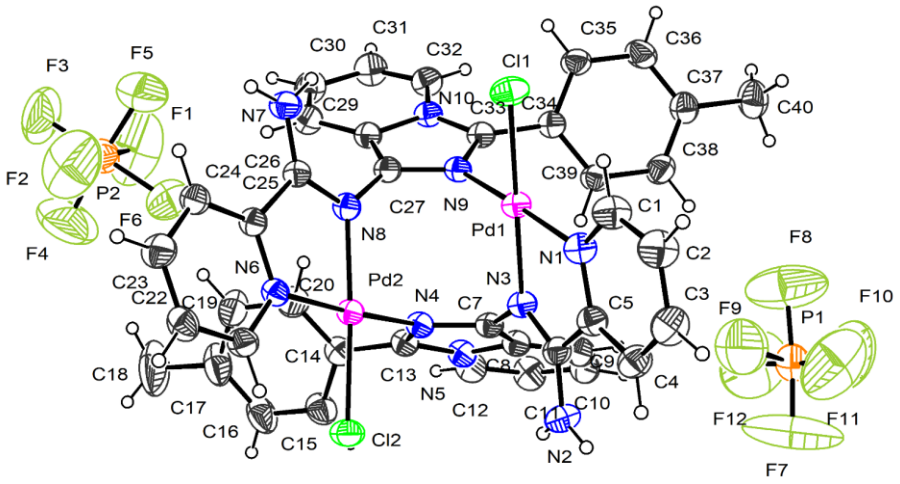


Figure S26. ORTEP diagram of **4**. Thermal ellipsoids are drawn at 30% probability level and solvents molecules were omitted for clarity.

Table S21: Bond lengths in **4**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.2865(13)	N6	C21	1.342(6)	C31	C32	1.329(8)
Pd1	N1	2.011(4)	N7	C26	1.300(6)	C34	C39	1.381(7)
Pd1	N3	2.017(4)	C5	C4	1.370(7)	C34	C35	1.386(7)
Pd1	N9	2.016(4)	C5	C6	1.479(7)	C39	C38	1.384(7)
Pd2	Cl2	2.2933(13)	C4	C3	1.383(8)	C38	C37	1.380(8)
Pd2	N4	2.011(4)	C3	C2	1.371(9)	C37	C36	1.391(8)
Pd2	N8	2.017(4)	C2	C1	1.375(8)	C37	C40	1.503(8)
Pd2	N6	2.006(4)	C27	C28	1.378(6)	C36	C35	1.381(8)
N1	C5	1.355(6)	C28	C29	1.404(7)	C9	C10	1.365(8)
N1	C1	1.341(7)	C33	C34	1.469(6)	C10	C11	1.409(9)
N3	C6	1.332(6)	C7	C8	1.377(6)	C11	C12	1.331(8)
N3	C7	1.401(6)	C8	C9	1.412(7)	C14	C20	1.370(8)
N2	C6	1.307(6)	C13	C14	1.465(7)	C14	C15	1.381(7)
N9	C27	1.371(6)	C25	C24	1.369(6)	C20	C19	1.369(9)
N9	C33	1.337(5)	C25	C26	1.500(6)	C19	C17	1.370(10)
N10	C28	1.409(6)	C24	C23	1.386(7)	C17	C16	1.383(11)
N10	C33	1.359(6)	C23	C22	1.361(8)	C17	C18	1.545(11)
N10	C32	1.399(6)	C22	C21	1.393(7)	C16	C15	1.372(9)
N5	C8	1.397(6)	N8	C27	1.401(5)	C29	C30	1.355(8)
N5	C13	1.369(6)	N8	C26	1.331(6)	C30	C31	1.428(9)
N5	C12	1.393(6)	N6	C25	1.361(6)	N4	C13	1.330(6)
N4	C7	1.368(6)						

Table S22: Bond angels in **4**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Pd1	Cl1	96.26(12)	C5	C4	C3	119.3(5)
N1	Pd1	N3	80.22(16)	C2	C3	C4	118.9(5)
N1	Pd1	N9	176.02(15)	C3	C2	C1	119.6(6)
N3	Pd1	Cl1	175.80(11)	N1	C1	C2	121.8(5)
N9	Pd1	Cl1	87.57(11)	N3	C6	C5	115.0(4)
N9	Pd1	N3	96.00(15)	N2	C6	N3	124.3(5)
N4	Pd2	Cl2	87.42(11)	N2	C6	C5	120.7(4)
N4	Pd2	N8	95.92(14)	N9	C27	N8	120.9(4)
N8	Pd2	Cl2	176.27(11)	N9	C27	C28	109.7(4)
N6	Pd2	Cl2	96.00(11)	C28	C27	N8	129.2(4)
N6	Pd2	N4	176.33(15)	C27	C28	N10	104.1(4)
N6	Pd2	N8	80.62(14)	C27	C28	C29	136.5(5)
C29	C28	N10	119.3(4)	C7	C8	C9	136.0(5)
N9	C33	N10	108.4(4)	N5	C13	C14	124.9(4)
N9	C33	C34	125.7(4)	N4	C13	N5	108.4(4)
N10	C33	C34	125.9(4)	N4	C13	C14	126.7(4)
N4	C7	N3	120.6(4)	N6	C25	C24	121.5(4)
N4	C7	C8	109.3(4)	N6	C25	C26	113.9(4)
C8	C7	N3	129.9(4)	C24	C25	C26	124.5(4)
N5	C8	C9	119.1(4)	C25	C24	C23	118.8(5)
C7	C8	N5	104.9(4)	C22	C23	C24	120.2(5)
C30	C29	C28	119.6(5)	C23	C22	C21	119.0(5)
C29	C30	C31	119.7(5)	N6	C21	C22	121.3(5)
C39	C34	C33	120.0(4)	C35	C34	C33	122.1(4)
C39	C34	C35	117.9(5)	C34	C39	C38	121.0(5)
C32	C31	C30	122.0(5)	C37	C38	C39	121.4(5)
C31	C32	N10	119.0(5)	C38	C37	C36	117.6(5)
C5	N1	Pd1	115.2(3)	C38	C37	C40	121.6(6)
C1	N1	Pd1	126.1(4)	C36	C37	C40	120.8(5)
C1	N1	C5	118.7(4)	C35	C36	C37	120.9(5)
C6	N3	Pd1	115.3(3)	C36	C35	C34	121.1(5)
C6	N3	C7	120.8(4)	C10	C9	C8	118.5(5)
C7	N3	Pd1	123.7(3)	C9	C10	C11	120.5(5)
C27	N9	Pd1	125.3(3)	C12	C11	C10	121.9(5)
C33	N9	Pd1	125.7(3)	C11	C12	N5	118.7(5)
C33	N9	C27	108.4(4)	C20	C14	C13	120.6(5)
C33	N10	C28	109.4(4)	C20	C14	C15	118.1(5)

C33	N10	C32	130.3(4)	C15	C14	C13	121.3(5)
C32	N10	C28	120.3(4)	C19	C20	C14	121.6(6)
C13	N5	C8	108.8(4)	C20	C19	C17	120.7(7)
C13	N5	C12	129.9(5)	C19	C17	C16	117.9(7)
C12	N5	C8	121.2(4)	C19	C17	C18	119.7(8)
C7	N4	Pd2	125.7(3)	C16	C17	C18	122.3(8)
C13	N4	Pd2	125.1(3)	C15	C16	C17	121.2(6)
C13	N4	C7	108.6(4)	C16	C15	C14	120.3(6)
C27	N8	Pd2	124.0(3)	N8	C26	C25	114.4(4)
C26	N8	Pd2	115.6(3)	N7	C26	N8	125.4(4)
C26	N8	C27	120.3(4)	N7	C26	C25	120.1(4)
C25	N6	Pd2	114.8(3)	N1	C5	C4	121.6(5)
C21	N6	Pd2	125.9(3)	N1	C5	C6	114.1(4)
C21	N6	C25	119.2(4)	C4	C5	C6	124.3(5)

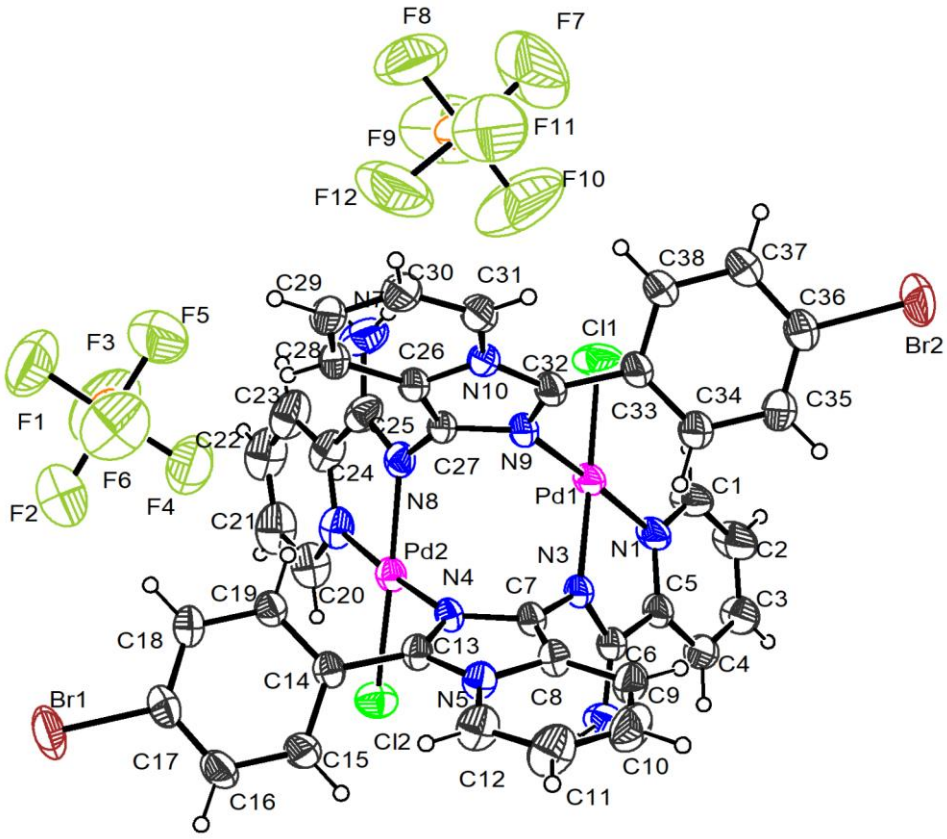


Figure S27. ORTEP diagram of **5**. Thermal ellipsoids are drawn at 30% probability level and solvents molecules were omitted for clarity.

Table S23: Bond lengths in **5**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.285(2)	C13	C14	1.472(7)	N8	C27	1.400(8)
Pd1	N1	2.024(5)	C14	C15	1.383(8)	N9	C27	1.363(7)
Pd1	N3	2.009(5)	C14	C19	1.381(8)	N9	C32	1.334(8)
Pd1	N9	2.030(5)	C15	C16	1.373(9)	N10	C26	1.390(8)
Pd2	Cl2	2.2914(18)	C16	C17	1.362(10)	N10	C31	1.391(8)
Pd2	N4	2.022(5)	C17	C18	1.364(9)	N10	C32	1.371(7)
Pd2	N6	2.027(6)	C18	C19	1.363(8)	C1	C2	1.385(10)
Pd2	N8	2.014(5)	C20	C21	1.396(11)	C2	C3	1.351(11)
Br1	C17	1.898(6)	C21	C22	1.369(14)	C3	C4	1.382(10)
Br2	C36	1.913(7)	C22	C23	1.362(14)	C4	C5	1.372(9)
N1	C1	1.332(8)	C23	C24	1.382(10)	C5	C6	1.482(8)
N1	C5	1.353(8)	C24	C25	1.463(11)	C7	C8	1.354(8)
N2	C6	1.300(8)	C26	C27	1.366(9)	C8	C9	1.421(9)
N3	C6	1.326(8)	C26	C28	1.434(8)	C9	C10	1.333(11)
N3	C7	1.402(7)	C28	C29	1.330(10)	C10	C11	1.428(12)
N4	C7	1.375(7)	C29	C30	1.417(11)	C11	C12	1.322(10)
N4	C13	1.337(7)	C30	C31	1.345(9)	C33	C38	1.376(9)
N5	C8	1.406(8)	C32	C33	1.470(9)	C34	C35	1.390(10)
N5	C12	1.393(8)	C33	C34	1.372(9)	C35	C36	1.353(11)
N5	C13	1.361(7)	N6	C24	1.361(10)	C36	C37	1.373(11)
N6	C20	1.333(10)	N7	C25	1.319(10)	C37	C38	1.386(10)
N8	C25	1.318(8)						

Table S24: Bond angels in **5**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Pd1	Cl1	96.26(16)	C18	C19	C14	121.3(6)
N1	Pd1	N9	175.1(2)	N6	C20	C21	120.6(9)
N3	Pd1	Cl1	174.36(16)	C22	C21	C20	119.4(9)
N3	Pd1	N1	80.0(2)	C23	C22	C21	119.7(8)
N3	Pd1	N9	95.56(19)	C22	C23	C24	119.6(10)
N9	Pd1	Cl1	88.36(15)	N6	C24	C23	120.7(8)
N4	Pd2	Cl2	88.63(14)	N6	C24	C25	114.1(6)
N4	Pd2	N6	175.4(2)	C23	C24	C25	125.2(8)
N6	Pd2	Cl2	95.93(19)	N7	C25	C24	119.4(7)
N8	Pd2	Cl2	176.05(16)	N8	C25	N7	124.3(8)
N8	Pd2	N4	95.3(2)	N8	C25	C24	116.2(7)
N8	Pd2	N6	80.1(2)	N10	C26	C28	118.8(6)
C1	N1	Pd1	125.8(5)	C27	C26	N10	105.3(5)

C1	N1	C5	119.2(6)	C27	C26	C28	135.8(6)
C5	N1	Pd1	114.9(4)	N9	C27	N8	121.2(5)
C6	N3	Pd1	116.1(4)	N9	C27	C26	109.7(6)
C6	N3	C7	117.9(5)	C26	C27	N8	129.0(5)
C7	N3	Pd1	125.6(4)	C29	C28	C26	118.6(7)
C7	N4	Pd2	125.1(4)	C28	C29	C30	121.4(6)
C13	N4	Pd2	126.8(4)	C31	C30	C29	121.4(7)
C13	N4	C7	107.7(5)	C30	C31	N10	118.3(7)
C12	N5	C8	121.3(5)	N9	C32	N10	108.4(5)
C13	N5	C8	108.3(5)	N9	C32	C33	125.8(6)
C13	N5	C12	130.4(5)	N10	C32	C33	125.5(6)
C20	N6	Pd2	125.9(6)	C34	C33	C32	120.7(6)
C20	N6	C24	119.9(7)	C34	C33	C38	119.4(6)
C24	N6	Pd2	114.1(5)	C38	C33	C32	119.8(6)
C25	N8	Pd2	115.2(5)	C33	C34	C35	120.3(7)
C25	N8	C27	119.6(6)	C36	C35	C34	118.9(7)
C27	N8	Pd2	125.2(4)	C35	C36	Br2	119.9(6)
C27	N9	Pd1	124.8(4)	C35	C36	C37	122.6(7)
C32	N9	Pd1	126.9(4)	C37	C36	Br2	117.5(6)
C32	N9	C27	108.1(5)	C36	C37	C38	117.7(7)
C26	N10	C31	121.5(5)	C33	C38	C37	121.1(7)
C32	N10	C26	108.4(5)	C7	C8	C9	136.5(6)
C32	N10	C31	130.1(6)	C10	C9	C8	119.3(7)
N1	C1	C2	121.0(7)	C9	C10	C11	120.8(7)
C3	C2	C1	120.3(7)	C12	C11	C10	121.6(7)
C2	C3	C4	118.8(7)	C11	C12	N5	118.7(7)
C5	C4	C3	119.4(7)	N4	C13	N5	108.8(5)
N1	C5	C4	121.3(6)	N4	C13	C14	125.2(5)
N1	C5	C6	114.1(5)	N5	C13	C14	125.6(5)
C4	C5	C6	124.6(6)	C15	C14	C13	119.9(6)
N2	C6	N3	125.2(6)	C19	C14	C13	121.6(5)
N2	C6	C5	120.2(6)	C19	C14	C15	118.4(5)
N3	C6	C5	114.6(5)	C16	C15	C14	120.7(7)
N4	C7	N3	120.8(5)	C17	C16	C15	118.9(6)
C8	C7	N3	129.1(5)	C16	C17	Br1	118.8(5)
C8	C7	N4	109.9(5)	C16	C17	C18	122.0(6)
N5	C8	C9	118.2(6)	C18	C17	Br1	119.2(5)
C7	C8	N5	105.3(5)	C19	C18	C17	118.8(6)

Table S1: **Optimization copper-free of copper-free Sonogashira reaction**

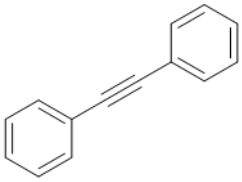
A 50 mL round bottom flask equipped with a magnetic stir bar was charged with the 4-bromotoluene (0.5 mmol), base (0.75 mmol), phenylacetylene (0.6 mmol), and catalyst **1** (0.5 mol%) in 10.0 mL absolute ethanol. Then it was stirred at specified temperature for a given time. Then, the reaction was allowed to cool to room temperature, ethyl acetate and H_2O were added and the layers were separated. The aqueous layer was extracted three times with ethylacetate, the combined organic layers were washed with water, dried over Na_2SO4, filtered, and concentrated in vacuo to yield the crude product, which was purified by preparative thin layer chromatography to produce the product.

General procedures for Sonogashira coupling reaction.

A 50 mL round bottom flask equipped with a magnetic stir bar was charged with the aryl bromide (1.0 eq.), K_2CO_3 (1.5 eq.), the terminal alkyne (1.2 eq.), catalyst **1** (0.5 mol%), and 10 mL absolute ethanol. Then it was stirred at 80 °C for 8 hours. The reaction was allowed to cool to room temperature, ethyl acetate and H_2O were added and the layers were separated. The aqueous layer was extracted three times with ethylacetate, the combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated in vacuo to yield the crude product, which was purified by preparative thin layer chromatography to yield the pure product (see specific procedures for individual purification conditions).

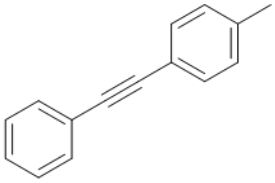
Specific procedures and characterization data for Sonogashira coupling products 3a-3p

1,2-diphenylethyne (3a)



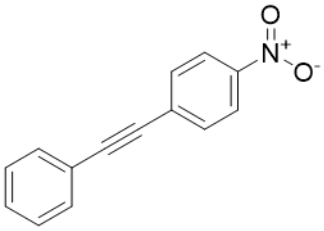
According to the general procedure, the reaction of bromobenzene (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 – 7.51 (m, 4H), 7.39 – 7.32 (m, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 132.6, 131.7, 128.5, 123.4, 89.5. NMR spectroscopic data matched literature values.[9]

1-methyl-4-(phenylethynyl)benzene (3b)



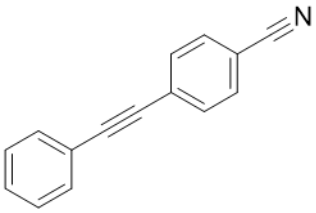
According to the general procedure, the reaction of 4-bromotoluene (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.50 (m, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.37 – 7.30 (m, 3H), 7.16 (d, *J* = 7.9 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.54, 131.70, 131.65, 129.26, 128.46, 128.22, 123.64, 120.3, 89.7, 88.8, 21.7. NMR spectroscopic data matched literature values.[9]

1-nitro-4-(phenylethynyl)benzene (3c)



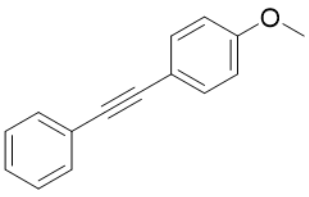
According to the general procedure, the reaction of 1-bromo-4-nitrobenzene (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 8.7 Hz, 2H), 7.67 (d, *J* = 8.7 Hz, 2H), 7.61 – 7.53 (m, 2H), 7.43 – 7.36 (m, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 147.1, 132.4, 132.0, 130.4, 129.4, 128.7, 123.8, 122.3, 94.8, 87.7. NMR spectroscopic data matched literature values.[9]

4-(phenylethynyl)benzonitrile (3d)



According to the general procedure, the reaction of 4-bromobenzonitrile (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 – 7.58 (m, 4H), 7.57 – 7.52 (m, 2H), 7.40 – 7.36 (m, *J* = 5.1, 1.8 Hz, 3H).^{13}C NMR (126 MHz, DMSO-d_6) δ 132.2, 132.2, 131.9, 129.3, 128.6, 128.4, 122.3, 118.7, 111.6, 93.9, 87.8. NMR spectroscopic data matched literature values.[10]

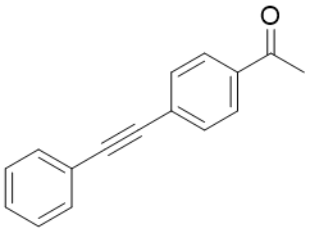
1-methoxy-4-(phenylethynyl)benzene (3e)



According to the general procedure, the reaction of 4-bromoanisole (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ

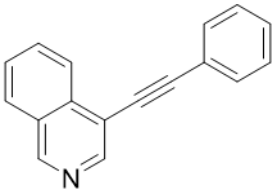
7.51 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.47 (d, *J* = 8.9 Hz, 2H), 7.38 – 7.29 (m, 3H), 6.88 (d, *J* = 8.9 Hz, 2H), 3.83 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 159.8, 133.2, 131.6, 128.4, 128.1, 123.7, 115.5, 114.1, 89.5, 88.2, 55.4. NMR spectroscopic data matched literature values.[9]

1-(4-(phenylethynyl)phenyl)ethan-1-one (3f)



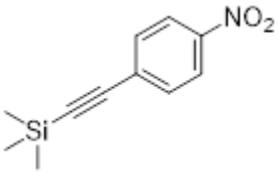
According to the general procedure, the reaction of 1-(4-bromophenyl)ethan-1-one (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 8.6 Hz, 2H), 7.55 (dd, *J* = 6.2, 3.4 Hz, 2H), 7.37 (td, *J* = 3.6, 3.2, 2.0 Hz, 3H), 2.62 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 197.3, 136.2, 131.8, 131.7, 128.8, 128.5, 128.3, 128.2, 122.7, 92.7, 88.6, 26.6. NMR spectroscopic data matched literature values.[9]

4-(phenylethynyl)isoquinoline (3g)



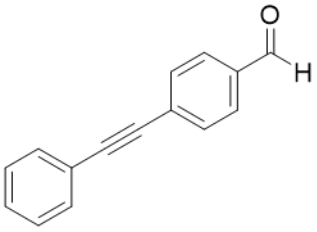
According to the general procedure, the reaction of 4-bromoisoquinoline (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.21 (s, 1H), 8.78 (s, 1H), 8.35 (d, *J* = 9.1 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.82 (ddd, *J* = 8.3, 6.9, 1.2 Hz, 1H), 7.72 – 7.62 (m, 3H), 7.45 – 7.35 (m, 3H). ^{13}C NMR (126 MHz, hloroform-*d*) δ 152.1, 146.6, 135.7, 131.9, 131.3, 129.0, 128.7, 128.1, 128.1, 128.0, 125.3, 123.0, 116.1, 96.9, 84.6. NMR spectroscopic data matched literature values.[11]

((p-Nitroxyphenyl)ethynyl)trimethylsilane (3h)



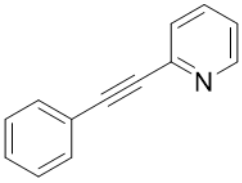
According to the general procedure, the reaction of 1-bromo-4-nitrobenzene (0.5 mmol), trimethylsilylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 8.6 Hz, 2H), 7.59 (d, *J* = 8.6 Hz, 2H), 0.27 (s, 9H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 147.3, 132.8, 130.1, 123.6, 102.9, 100.8, -0.15. NMR spectroscopic data matched literature values.[12]

4-(Phenylethynyl)benzaldehyde (3i)



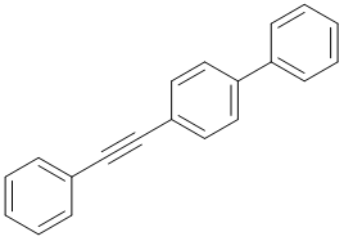
According to the general procedure, the reaction of 4-bromobenzaldehyde (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.02 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.60 – 7.53 (m, 2H), 7.38 (p, *J* = 3.1, 2.6 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 191.6, 135.5, 132.2, 131.9, 129.7, 129.7, 129.1, 128.6, 122.6, 93.6, 88.6. NMR spectroscopic data matched literature values.[10]

2-(phenylethynyl) pyridine (3j)



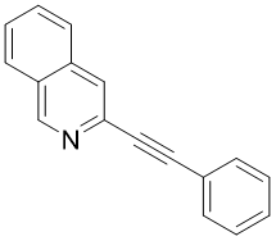
According to the general procedure, the reaction of 2-bromopyridine (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57 (d, *J* = 4.7 Hz, 1H), 7.65 – 7.54 (m, 3H), 7.47 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.28 (m, 3H), 7.21 – 7.14 (m, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.1, 143.5, 136.2, 132.1, 129.0, 128.4, 127.2, 122.8, 122.28, 89.3, 88.7. NMR spectroscopic data matched literature values.[13]

4-(phenylethynyl)-1,1'-biphenyl (3k)



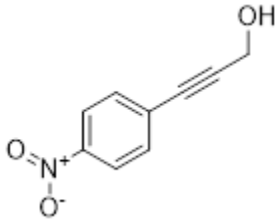
According to the general procedure, the reaction of 4-bromobiphenyl (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 (dd, *J* = 8.9, 1.4 Hz, 6H), 7.57 (dd, *J* = 7.6, 2.1 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.40 – 7.34 (m, 4H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 141.1, 140.5, 132.2, 131.8, 129.0, 128.5, 128.4, 127.8, 127.2, 123.4, 122.3, 90.2, 89.4. NMR spectroscopic data matched literature values.[10]

3-(phenylethynyl)isoquinoline (3l)



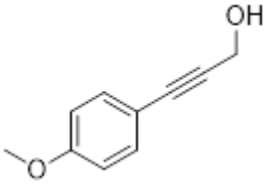
According to the general procedure, the reaction of 3-bromoisoquinoline (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.00 (s, 1H), 8.22 (s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.72 (m, *J* = 8.0, 3.7 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.58 (dd, *J* = 5.2, 2.6 Hz, 2H), 7.53 – 7.48 (m, 1H), 7.38 – 7.32 (m, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 152.1, 146.8, 138.20 131.7, 130.0, 129.4, 128.8, 128.5, 127.6, 127.2, 127.2, 122.6, 117.4, 86.7. HRMS (ESI) calculated for $[C_{17}H_{11}N+H]^+$: 230.0965, found 230.0960.

3-(4-nitrophenyl) prop-2-yn-1-ol (3m)



According to the general procedure, the reaction of 1-bromo-4-nitrobenzene (0.5 mmol), propargyl alcohol (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 (d, *J* = 8.9 Hz, 2H), 7.57 (d, *J* = 8.9 Hz, 2H), 4.54 (s, 2H), 1.86 (s, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 147.4, 132.6, 129.6, 123.7, 92.6, 83.96, 51.6. NMR spectroscopic data matched literature values.[14]

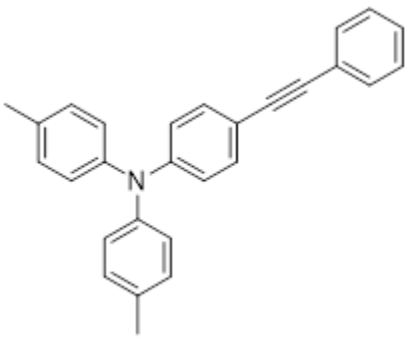
3-(4-methoxyphenyl)prop-2-yn-1-ol (3n)



According to the general procedure, the reaction of 4-bromoanisole (0.5 mmol), propargyl alcohol (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.9 Hz, 2H), 4.47 (s, 2H), 3.79 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 159.8, 133.3, 114.7, 114.0, 86.0, 85.7, 55.4, 51.7. NMR spectroscopic data matched literature values.[14]

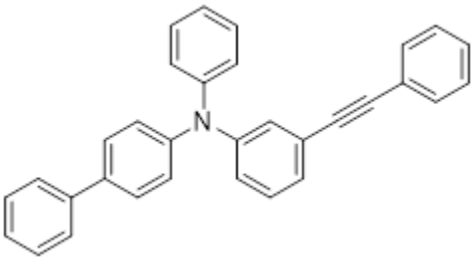
4-methyl-N-(4-(phenylethynyl)phenyl)-N-(p-tolyl)aniline (3o)

According to the general procedure, the reaction of 4-bromo-N,N-di-p-tolylaniline (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound as light yellow solid after work-up and chromatography.



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.36 – 7.30 (m, 5H), 7.09 (d, *J* = 8.8 hz, 4H), 7.01 (d, *J* = 8.8 hz, 4H), 6.94 (d, *J* = 8.7 Hz, 2H), 2.32 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.4, 144.8, 133.4, 132.5, 131.57, 130.2, 128.4, 127.9, 125.3, 124.8, 121.2, 115.2, 90.0, 88.4, 21.0. HRMS (ESI) calculated for $[C_{28}H_{23}N+H]^{+}$: 347.1904, found 347.1904.

N-phenyl-N-(3-(phenylethynyl)phenyl)-[1,1'-biphenyl]-4-amine (3p)



According to the general procedure, the reaction of N-(3-bromophenyl)-N-phenyl-[1,1'-biphenyl]-4-amine (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%) in ethanol for 8 h at 80 °C, affording the title compound as light yellow solid after work-up and chromatography and ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.55 (m, 2H), 7.50 (td, *J* = 6.0, 5.4, 3.3 Hz, 4H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.26 (m, 7H), 7.25 – 7.18 (m, 2H), 7.18 – 7.13 (m, 4H), 7.13 – 7.05 (m, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.9, 147.5, 147.0, 140.7, 135.7, 131.7, 129.6, 129.5, 128.9, 128.5, 128.4, 128.1, 127.0, 126.9, 126.8, 126.1, 124.8, 124.4, 124.3, 123.4, 89.6, 89.3. HRMS (ESI) calculated for $[C_{32}H_{23}N+H]^{+}$: 422.1904, found 422.1866.

Hot filtration test

Bromotoluene (0.5 mmol), phenylacetylene (0.6 mmol), K_2CO_3 (0.75 mmol), catalyst **1** (0.5 mol%), and ethanol (10.0 mL) was stirred at 80 ºC. After 2 hours, the reaction mixture was filtered through a short pad of celite in hot condition and again stirred for next 6 h. After completion of the reaction, the mixture was cooled, diluted with ethyl acetate (30.0 mL). Then it was filtered through a short pad of celite and filtrate was removed under reduced pressure. The crude product was purified by preparative thin layer chromatography and the yield of product (**3b**) was 88%.

Optimization of C–P bond formation reaction

4-iodoanisole (0.5 mmol eq.), base (0.75 mmol.), diethylphosphite (0.6mmol), and catalyst (0.5 mol%) were taken in 10.0 mL solvent. Then it was stirred at specified temperature for a given time. The reaction was allowed to cool to room temperature, solvent was removed. Then, ethyl

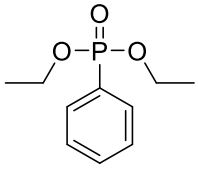
acetate and H_2O were added and the layers were separated. The aqueous layer was extracted three times with ethylacetate, the combined organic layers were washed with water, dried over Na_2SO4, filtered, and concentrated in vacuo to yield the crude product, which was purified by preparative thin layer chromatography to obtain isolated yield.

General procedure for C–P bond formation reaction

Arylhalide (1.0 mmol eq.), base (1.5 mmol.), diethylphosphite (1.2 mmol), and catalyst **1** (0.5 mol%) were taken in 10.0 mL ethanol. Then it was stirred at 80 °C for 10 hours. The reaction was allowed to cool to room temperature, solvent was removed. Then, ethyl acetate and H_2O were added and the layers were separated. The aqueous layer was extracted three times with ethylacetate, the combined organic layers were washed with water, dried over Na_2SO4, filtered, and concentrated in vacuo to yield the crude product, which was purified by preparative thin layer chromatography to obtain isolated yield of pure product.

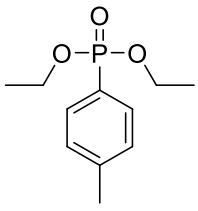
Specific procedures and characterization data for C–P coupling products 5a–5e

Diethyl phenylphosphonate (5a)



According to the general procedure, the reaction of iodobenzene (1.0 mmol), diethylphosphite (1.2 mmol), KOH (1.5 mmol), catalyst **1** (0.5 mol%) in ethanol for 10 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (dd, *J* = 13.3, 7.4 Hz, 2H), 7.53 (d, *J* = 6.8 Hz, 1H), 7.48 – 7.42 (m, 2H), 4.10 (dt, *J* = 18.2, 7.3 Hz, 4H), 1.31 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 132.56, 131.91, 131.82, 128.67, 128.52, 127.37, 62.27, 16.45. ^{31}P NMR (162 MHz, Chloroform-*d*) δ 18.84. NMR spectroscopic data were in congruent with literature values. [15]

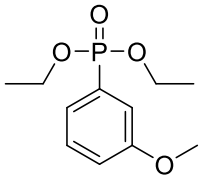
Diethyl (4-meylphenyl)phosphonate (5b)



According to the general procedure, the reaction of 4-iodotoluene (1.0 mmol), diethylphosphite (1.2 mmol), KOH (1.5 mmol), catalyst **1** (0.5 mol%) in ethanol for 10 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (dd, *J* = 13.2, 7.9 Hz, 2H), 7.22 – 7.18 (m, 2H), 4.00 (dd, *J* = 17.6, 10.5 Hz, 4H), 2.33 (s, 3H), 1.24 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.12, 131.96, 129.26, 62.20, 21.74, 16.43. ^{31}P NMR

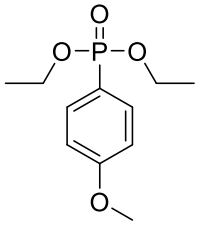
(243 MHz, Chloroform-*d*) δ 19.56. NMR spectroscopic data were in congruent with literature values. [15]

Diethyl (3-methoxyphenyl)phosphonate (5c)



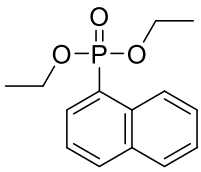
According to the general procedure, the reaction of 3-iodoanisole (1.0 mmol), diethylphosphite (1.2 mmol), KOH (1.5 mmol), catalyst **1** (0.5 mol%) in ethanol for 10 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.21 (m, 3H), 6.99 (dt, *J* = 5.8, 2.6 Hz, 1H), 4.10 – 3.94 (m, 4H), 3.75 (s, 3H), 1.23 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.61, 130.54, 129.91, 129.74, 128.69, 124.06, 123.97, 118.84, 116.50, 116.39, 62.21, 55.48, 16.42. ^{31}P NMR (162 MHz, Chloroform-*d*) δ 18.65. NMR spectroscopic data were in congruent with literature values. [16]

Diethyl (4-methoxyphenyl)phosphonate (5d)



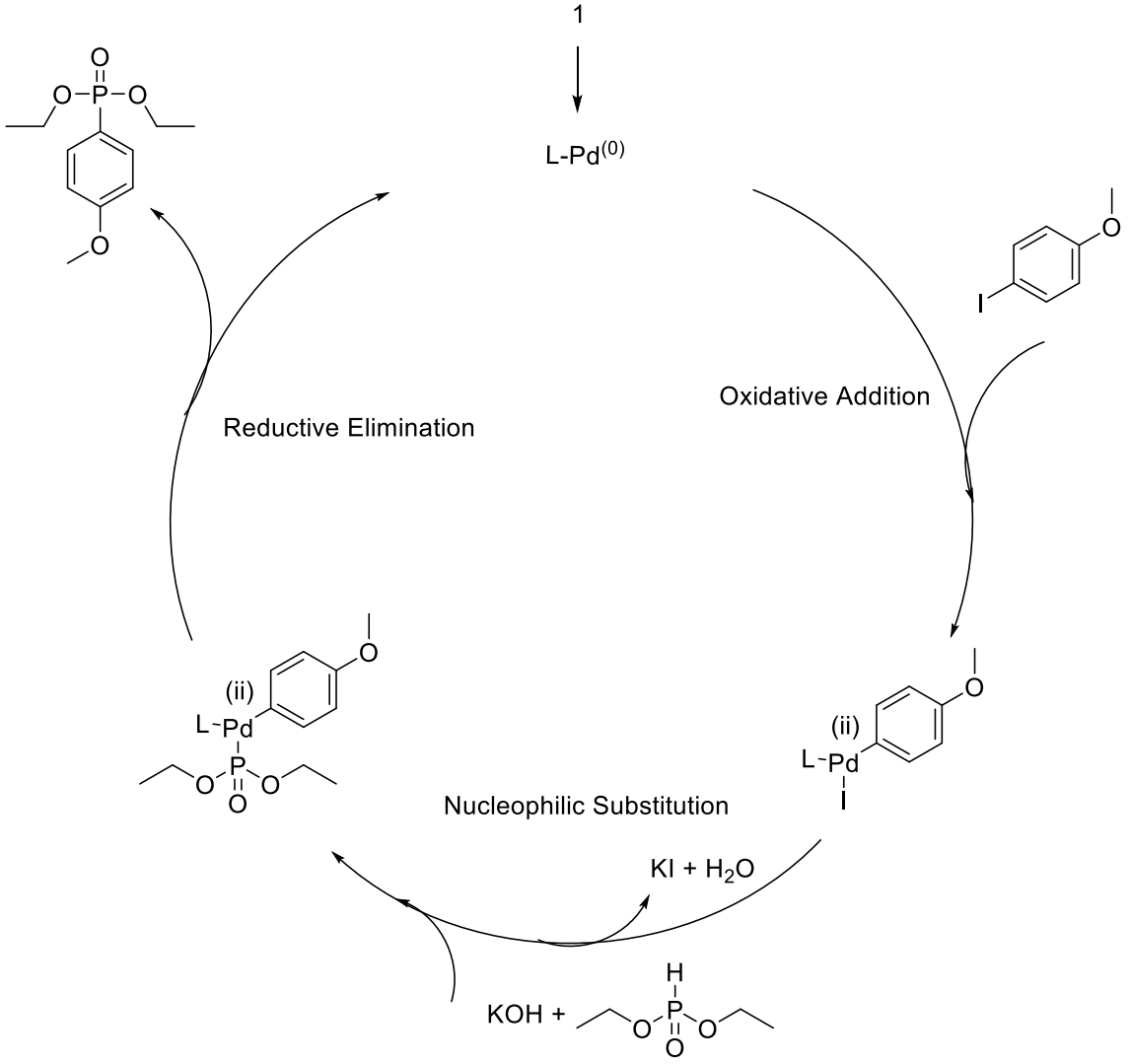
According to the general procedure, the reaction of 4-iodoanisole (1.0 mmol), diethylphosphite (1.2 mmol), KOH (1.5 mmol), catalyst **1** (0.5 mol%) in ethanol for 10 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.76 – 7.69 (m, 2H), 6.96 (dd, *J* = 8.7, 3.3 Hz, 2H), 4.14 – 3.99 (m, 4H), 3.85 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 162.99, 133.93, 133.86, 118.89, 114.22, 114.11, 62.12, 62.08, 55.48, 16.47, 16.42. ^{31}P NMR (243 MHz, Chloroform-*d*) δ 19.73. NMR spectroscopic data were in congruent with literature values.[17]

Diethyl naphthalen-1-ylphosphonate (5e)



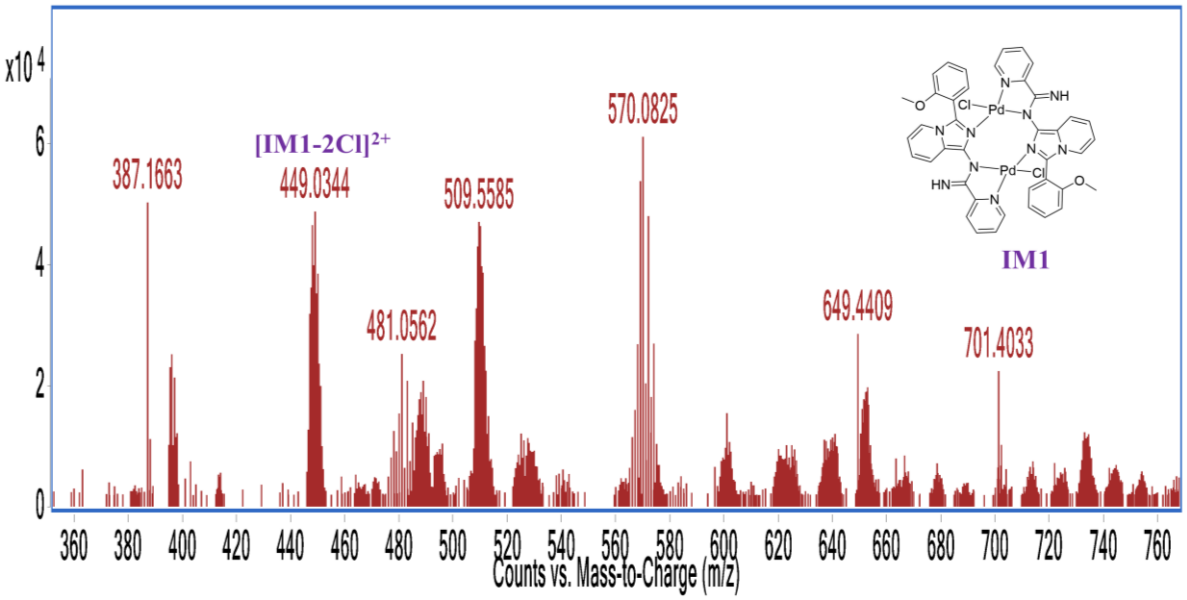
According to the general procedure, the reaction of 1-iodonaphthalene (1.0 mmol), diethylphosphite (1.2 mmol), KOH (1.5 mmol), catalyst **1** (0.5 mol%) in ethanol for 10 h at 80 °C, affording the title compound after work-up and chromatography. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.51 (d, *J* = 8.5 Hz, 1H), 8.24 (dd, *J* = 16.3, 7.0 Hz, 1H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.57 – 7.51 (m, 2H), 4.25 – 4.16 (m, 2H), 4.08 (dd, *J* = 17.6, 7.6 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 134.86, 134.77, 133.80, 133.77, 128.90, 127.55,

126.80, 126.49, 124.75, 124.59, 123.78, 62.31, 16.50. ^{31}P NMR (162 MHz, Chloroform-*d*) δ 19.20. NMR spectroscopic data were in congruent with literature values. [18]

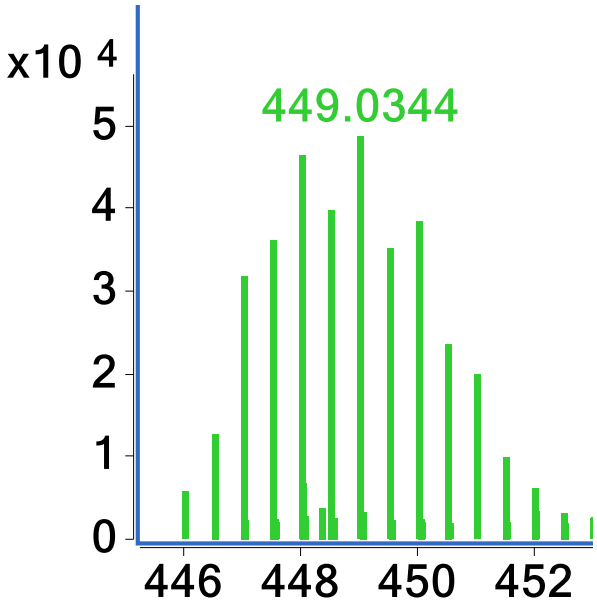


Scheme S1: Proposed mechanishm for C-P bond formation between 4-iodoanisole and diethylphosphite catalyzed by catalyst **1**.

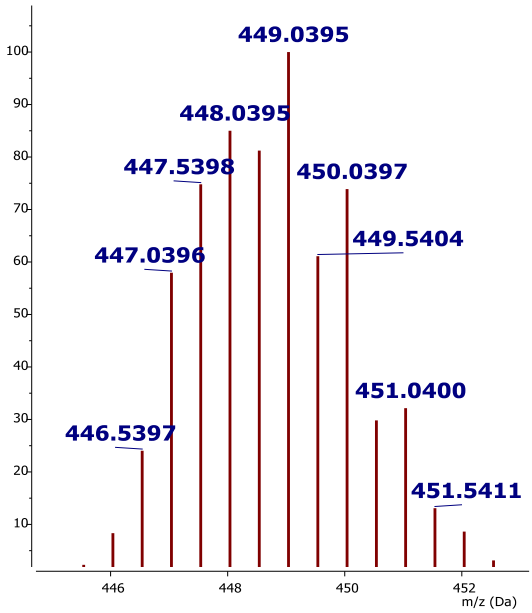
HRMS analysis of Sonogashira coupling Intermediates



(a)

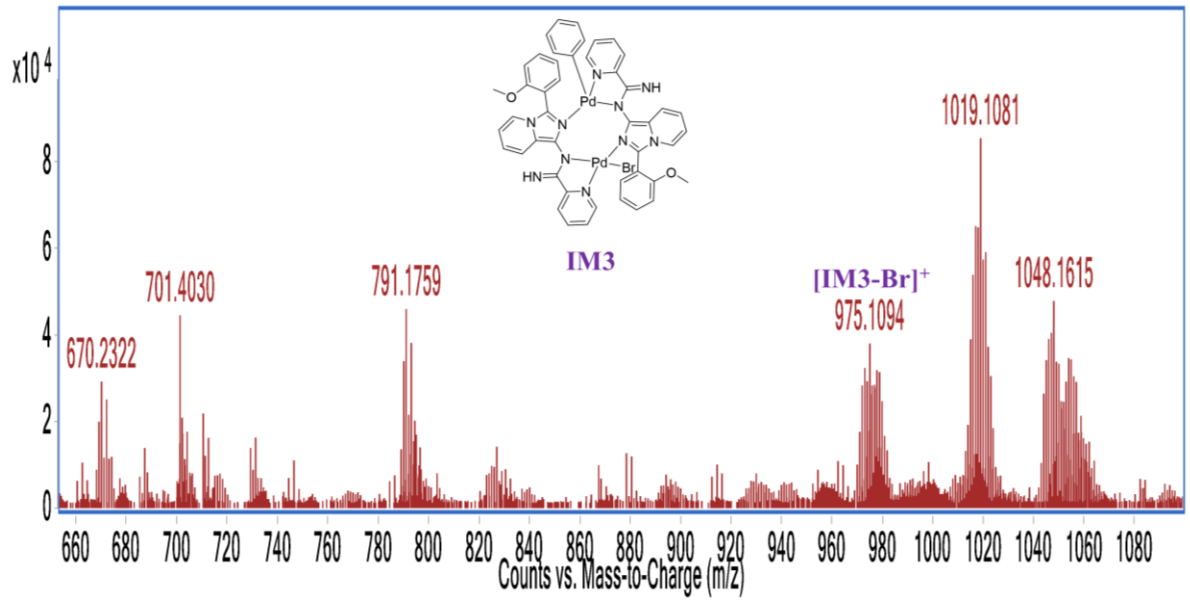


(b)

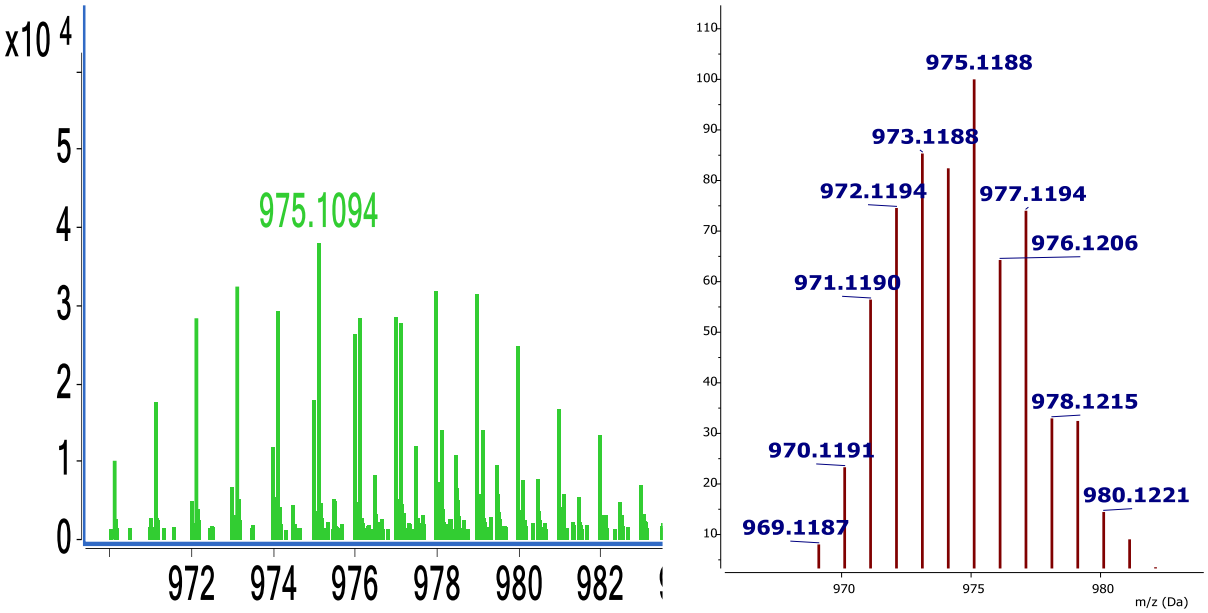


(c)

Figure S28: HRMS (ESI) spectra of intermediate IM1. (a) full, (b) expanded, and (c) simulated spectra at *m/z* 449.0344

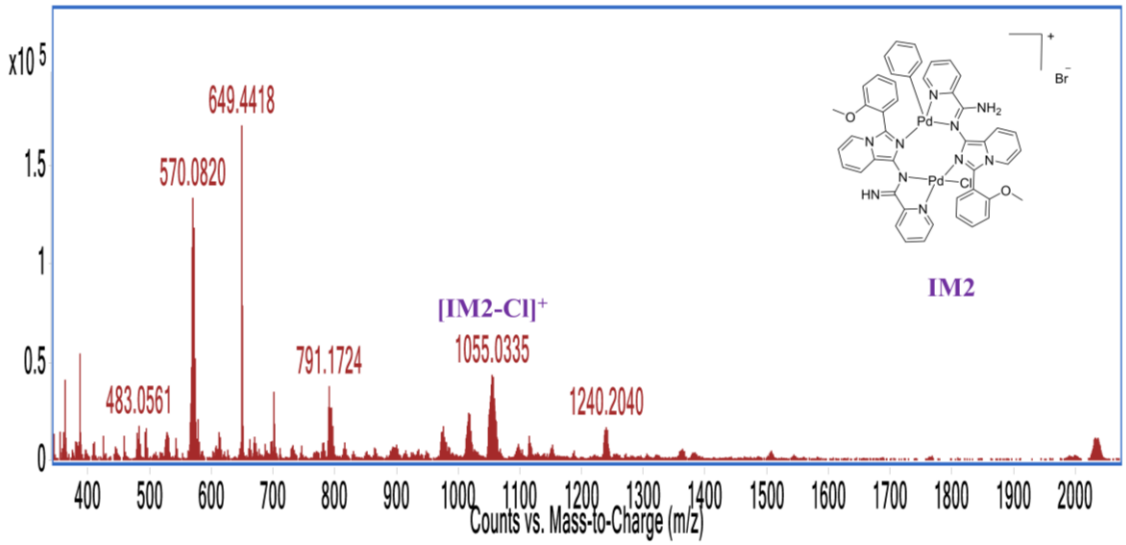


(a)

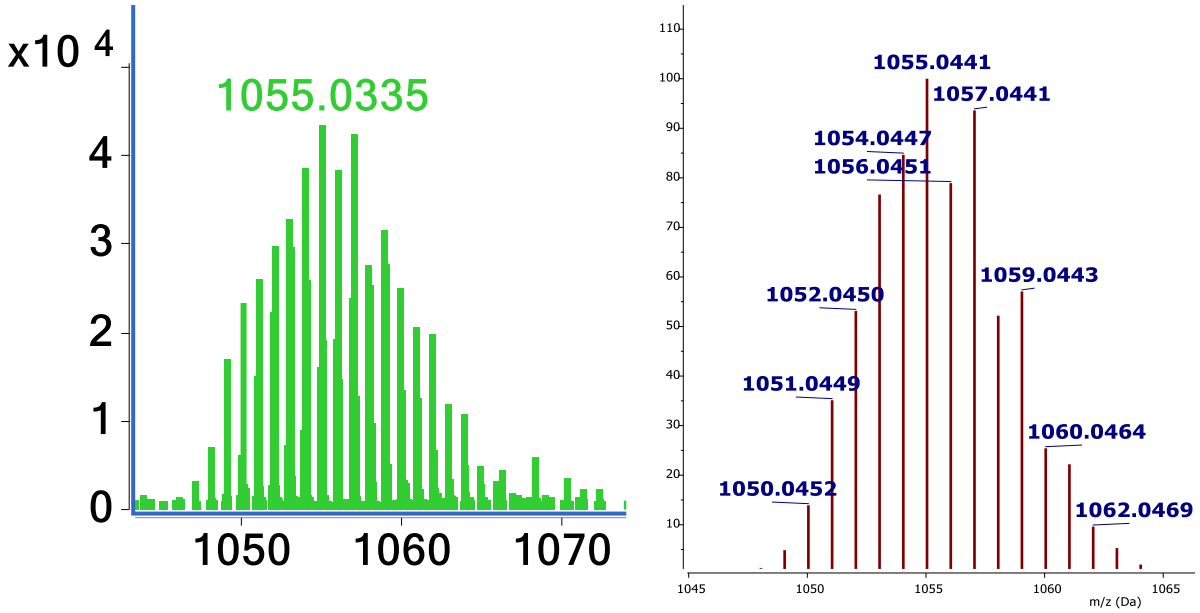


(b) **(c)**

Figure S29: HRMS (ESI) spectra of intermediate IM1. (a) full, (b) expanded, and (c) simulated spectra at *m/z* 975.1094.

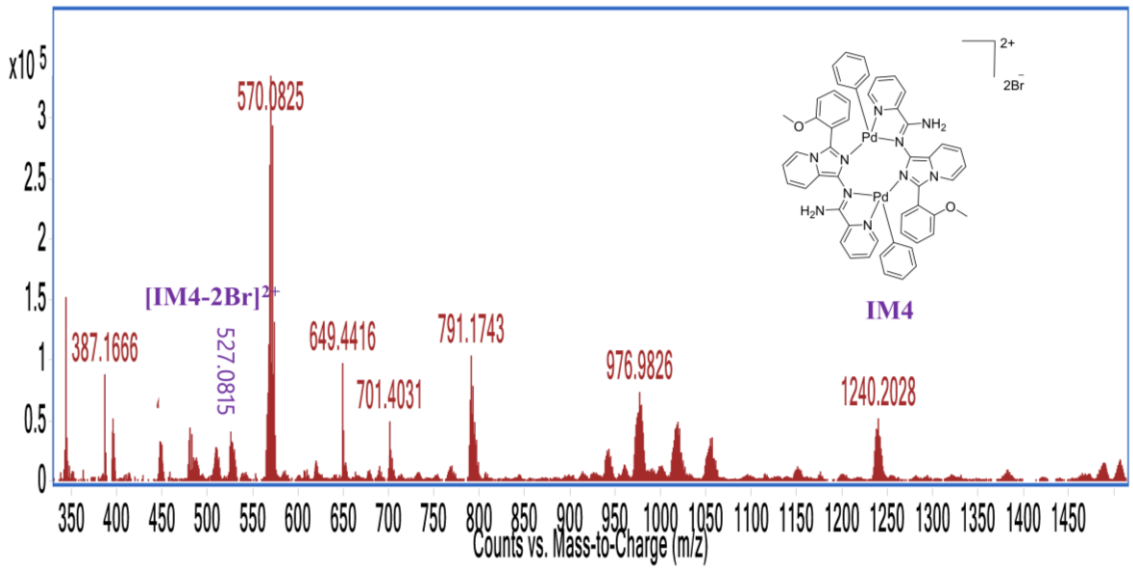


(a)

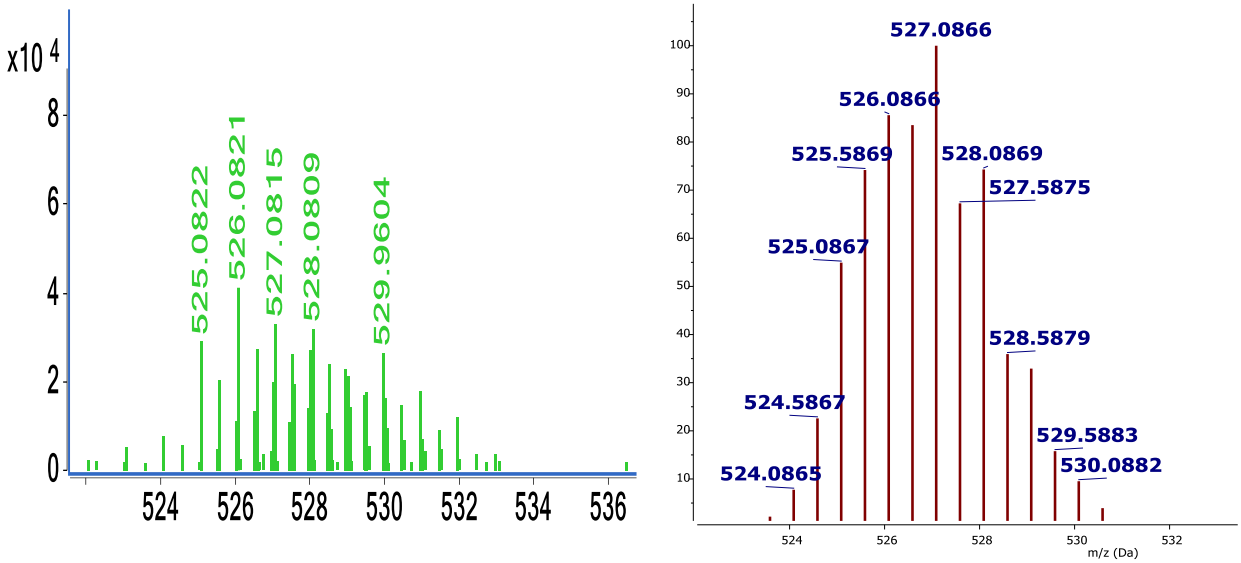


(b) (c)

Figure S30: HRMS (ESI) spectra of intermediate IM1. (a) full, (b) expanded, and (c) simulated spectra at *m/z* 1055.0355.



(a)

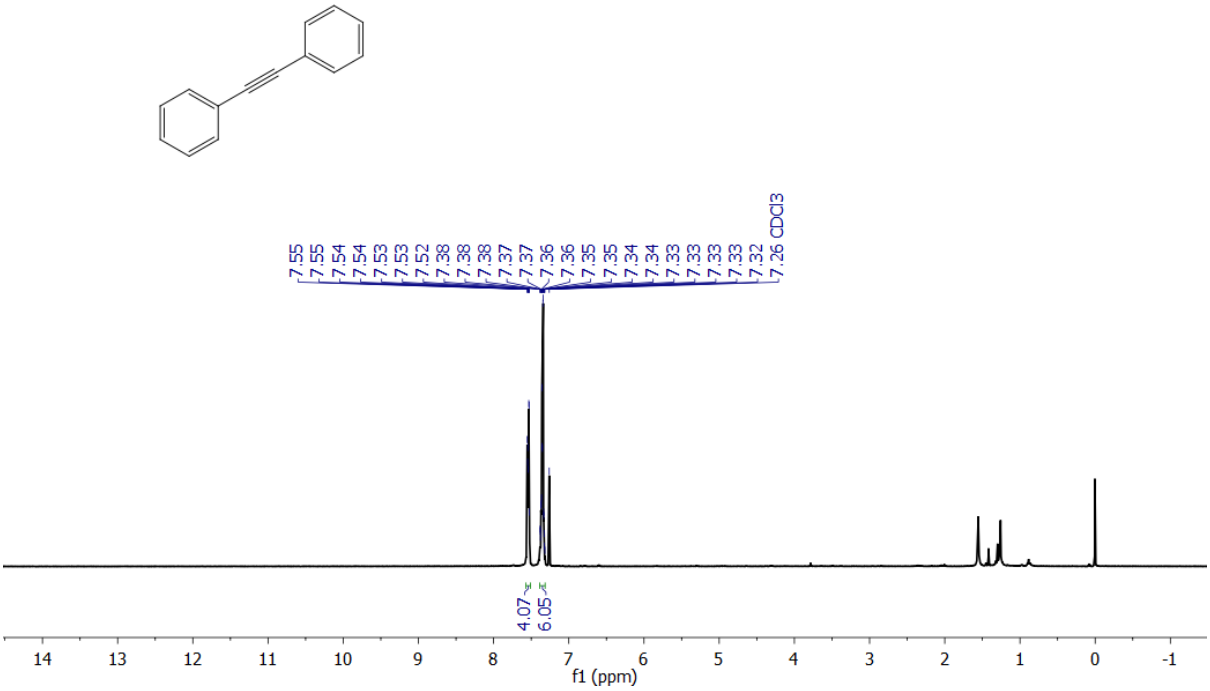


(b) **(c)**

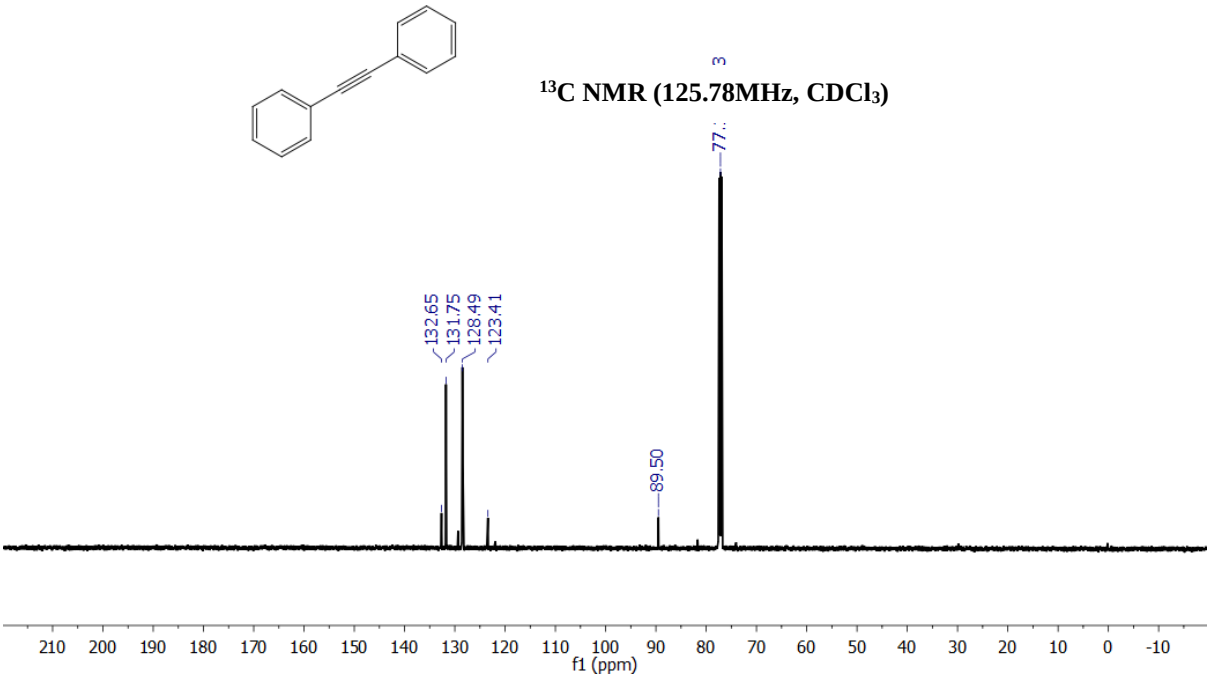
Figure S31: HRMS (ESI) spectra of intermediate IM1. (a) full, (b) expanded, and (c) simulated spectra at *m/z* 527.0821.

NMR spectra of Catalytic products:

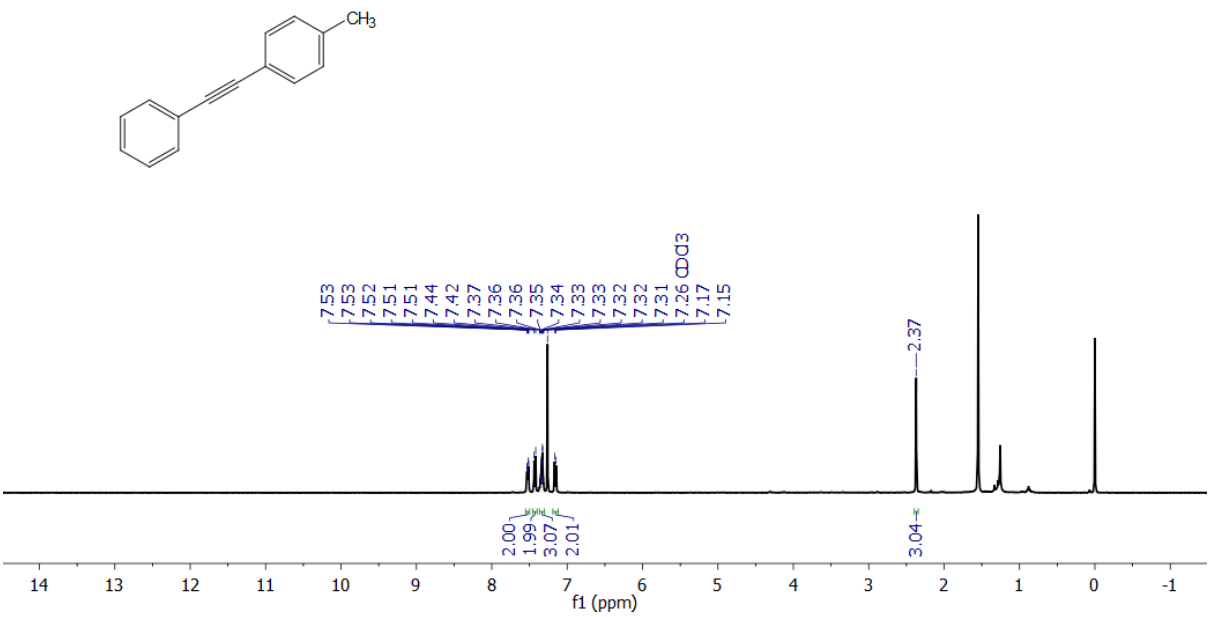
^{1}H NMR (400MHz, $CDCl_3$)



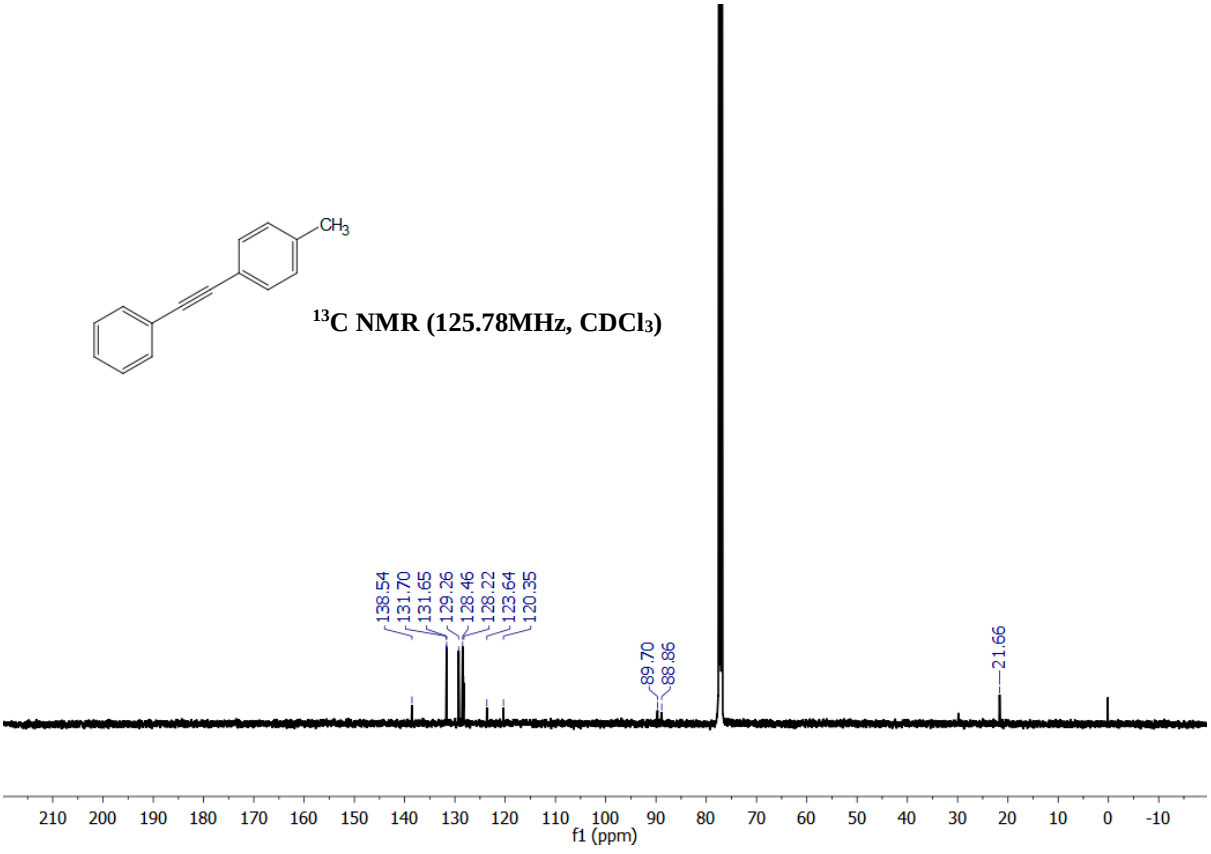
^{13}C NMR (125.78MHz, $CDCl_3$)



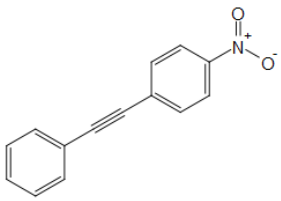
^{1}H NMR (400MHz, $CDCl_3$)

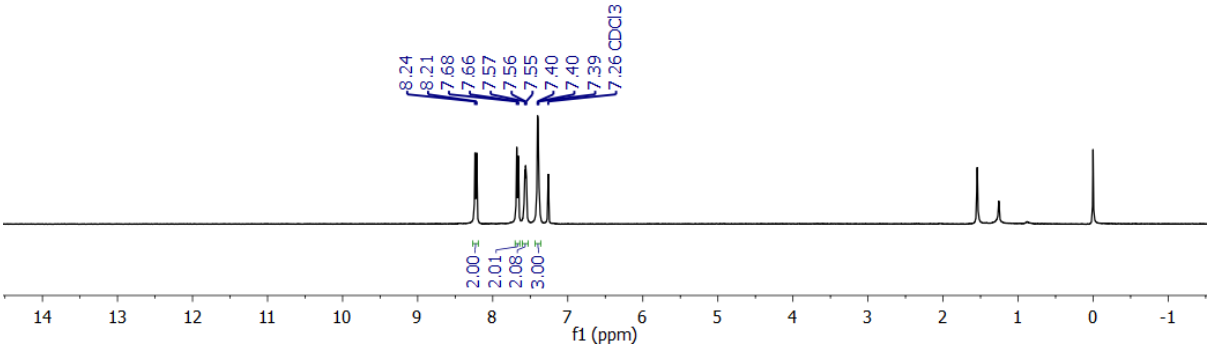


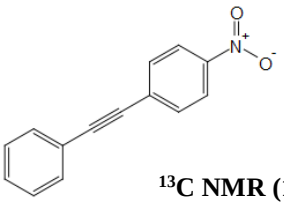
^{13}C NMR (125.78MHz, $CDCl_3$)



^{1}H NMR (400MHz, $CDCl_3$)

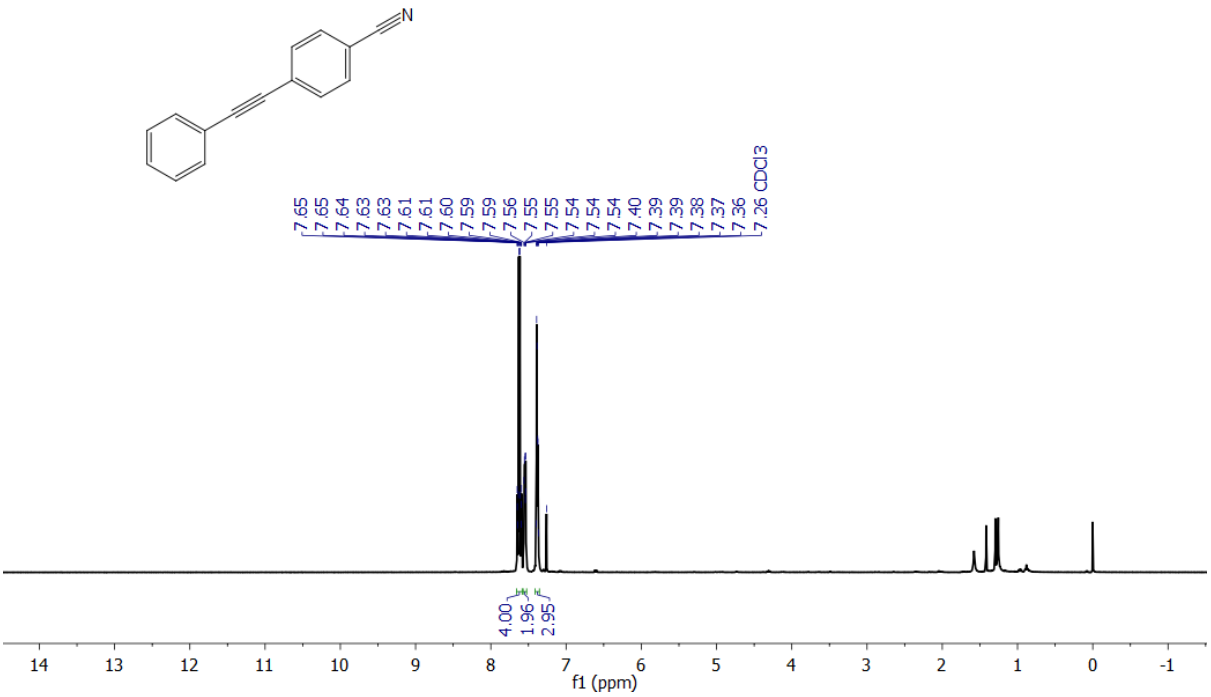




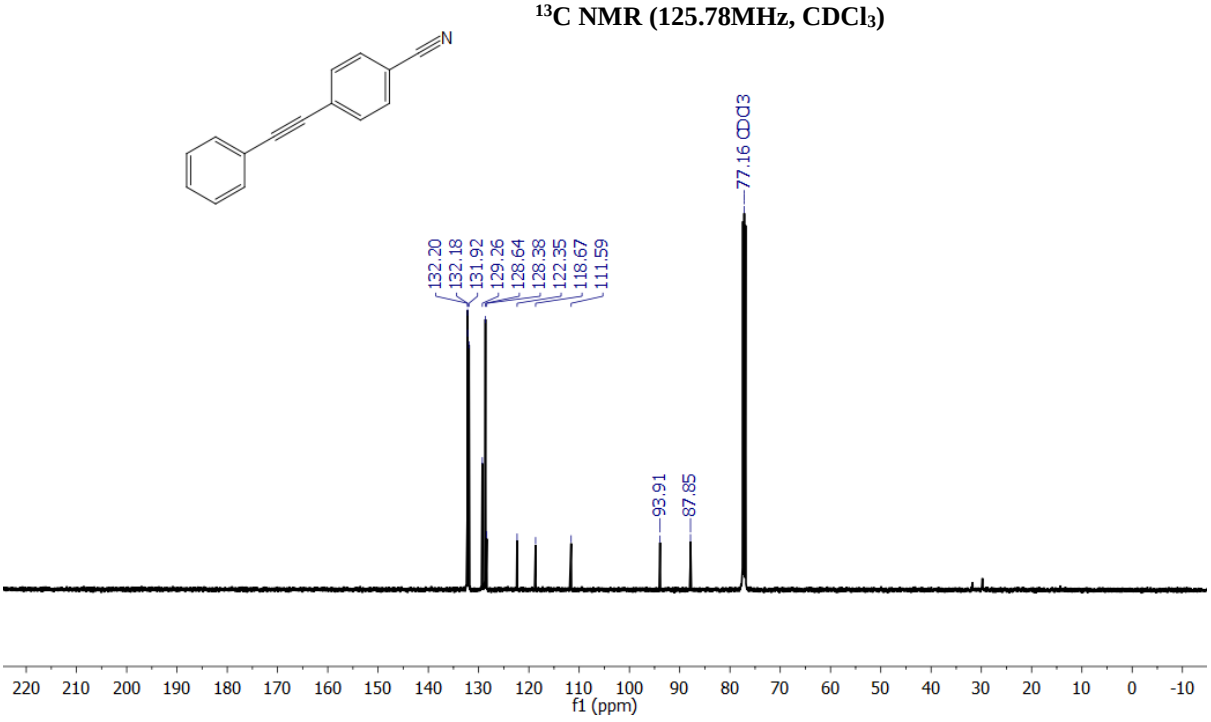


^{13}C NMR (125.78MHz, $CDCl_3$)

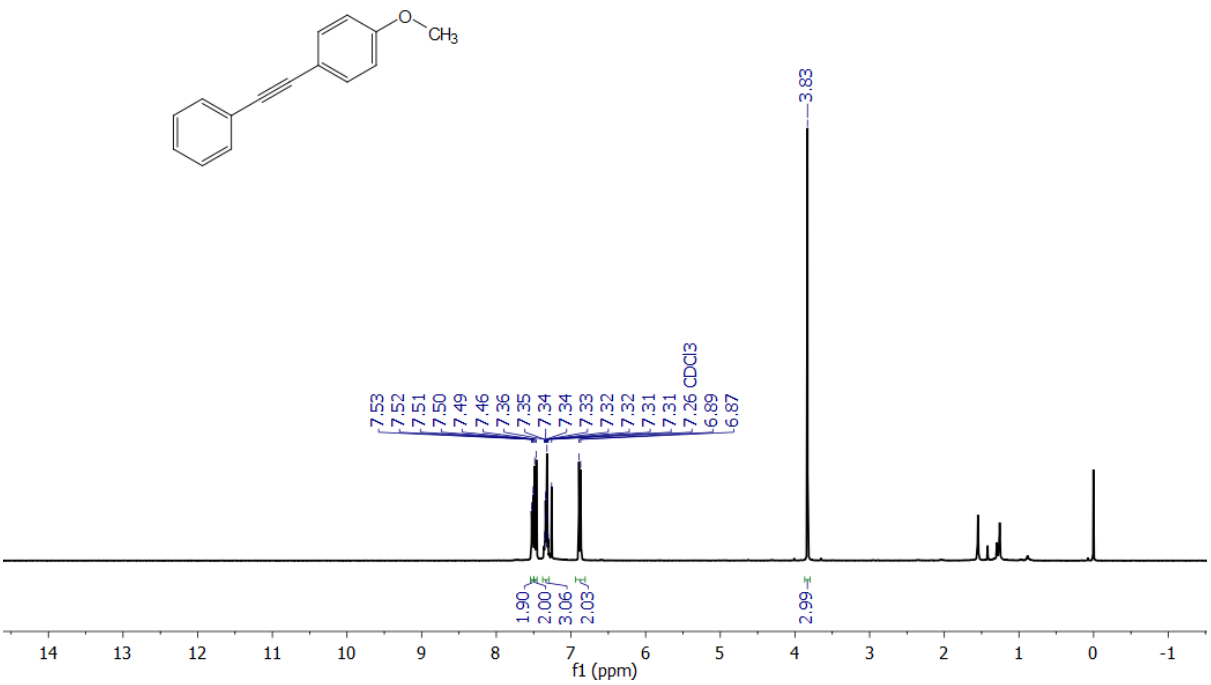
^{1}H NMR (400MHz, $CDCl_3$)

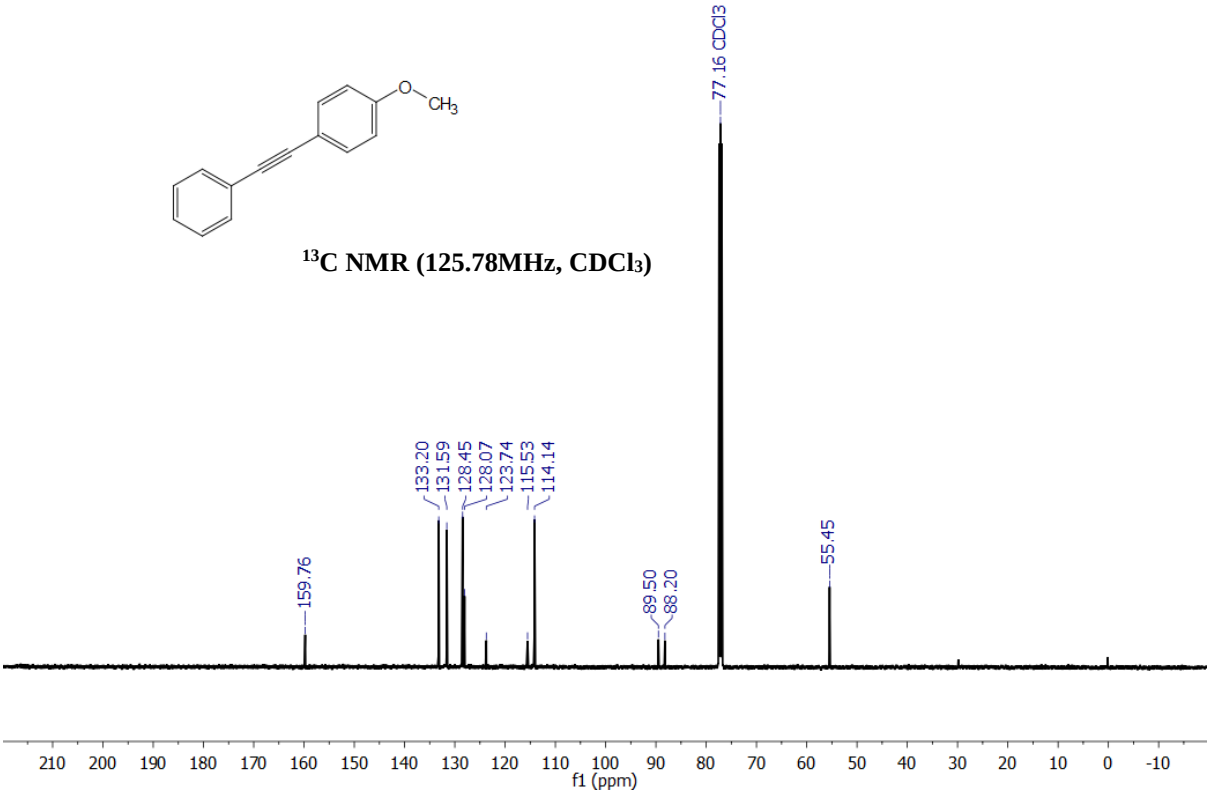


^{13}C NMR (125.78MHz, $CDCl_3$)



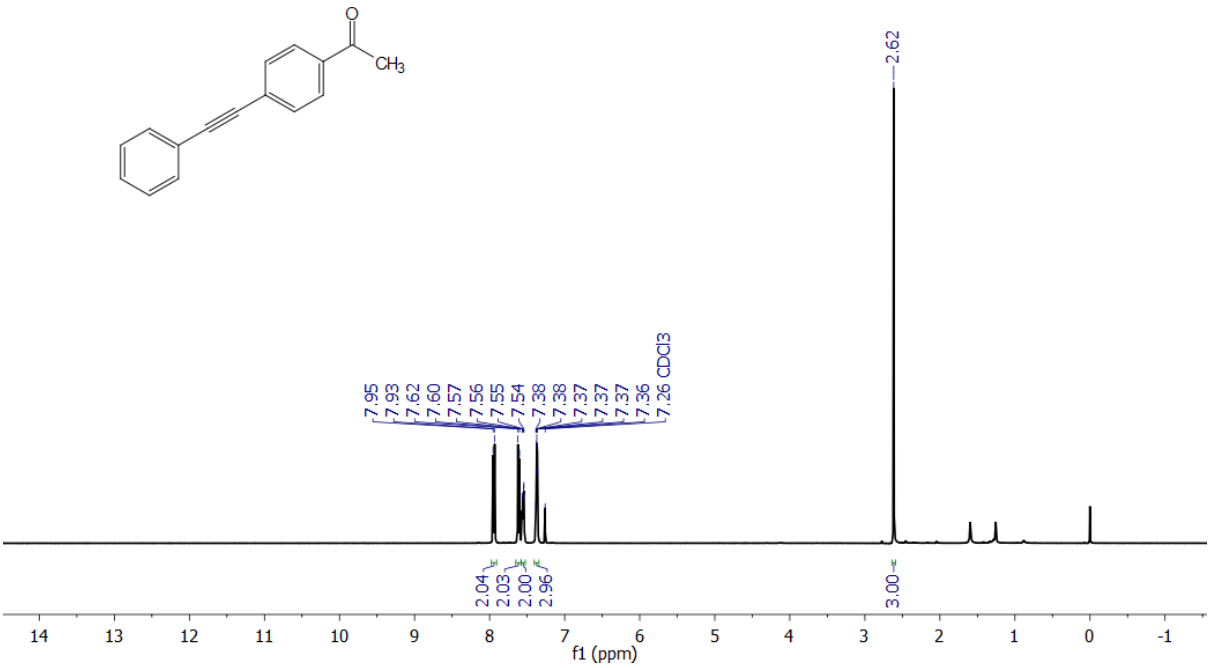
^{1}H NMR (400MHz, $CDCl_3$)



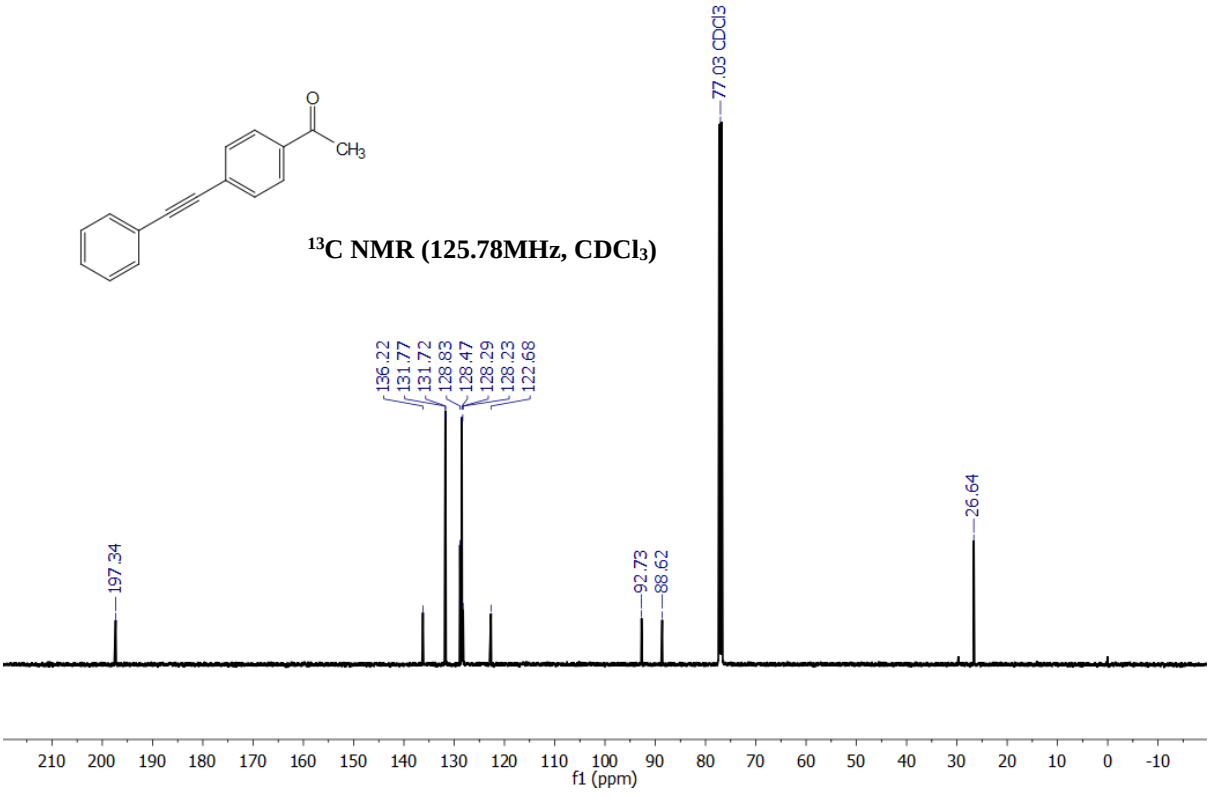


^{13}C NMR (125.78MHz, $CDCl_3$)

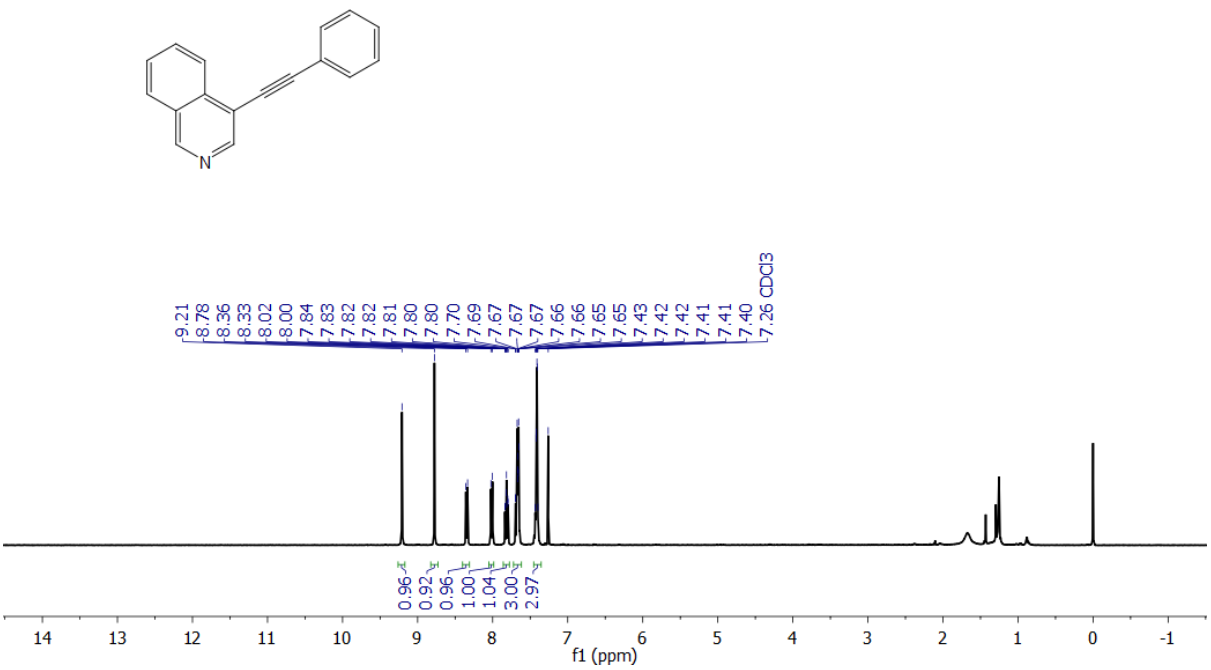
^{1}H NMR (400MHz, $CDCl_3$)



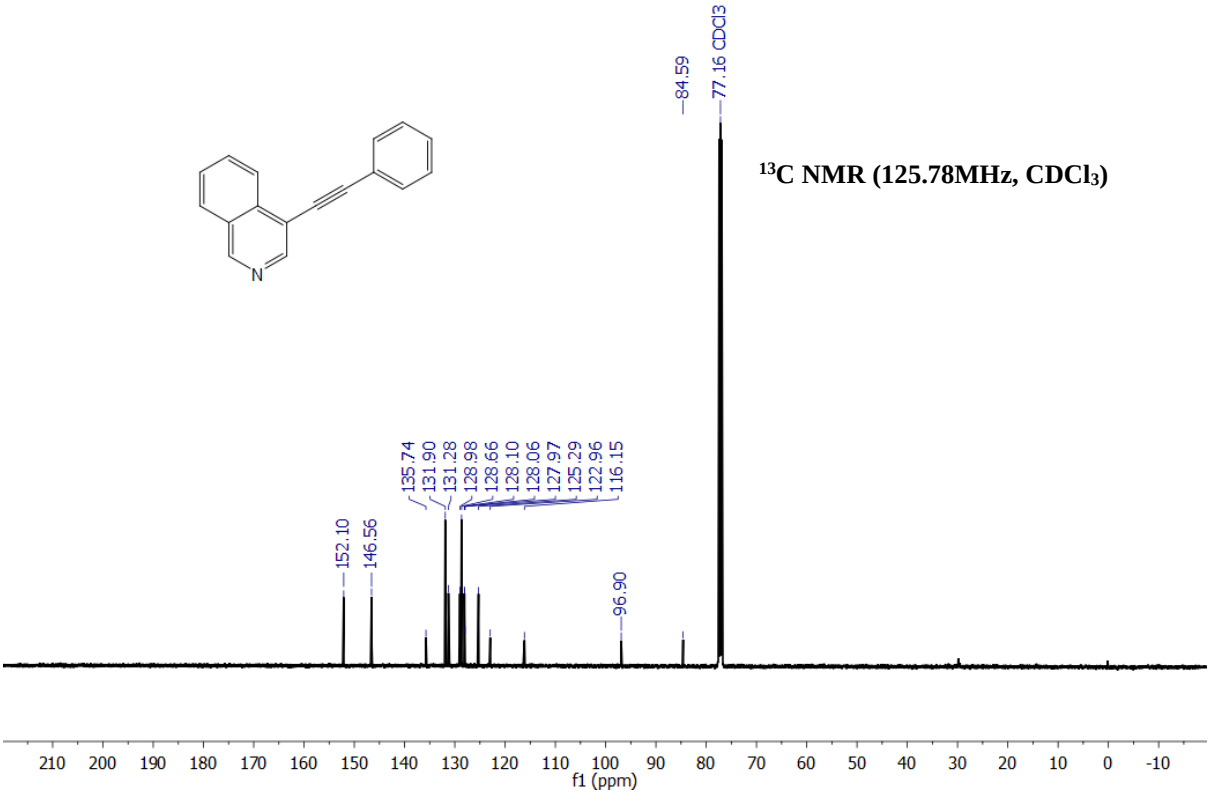
^{13}C NMR (125.78MHz, $CDCl_3$)



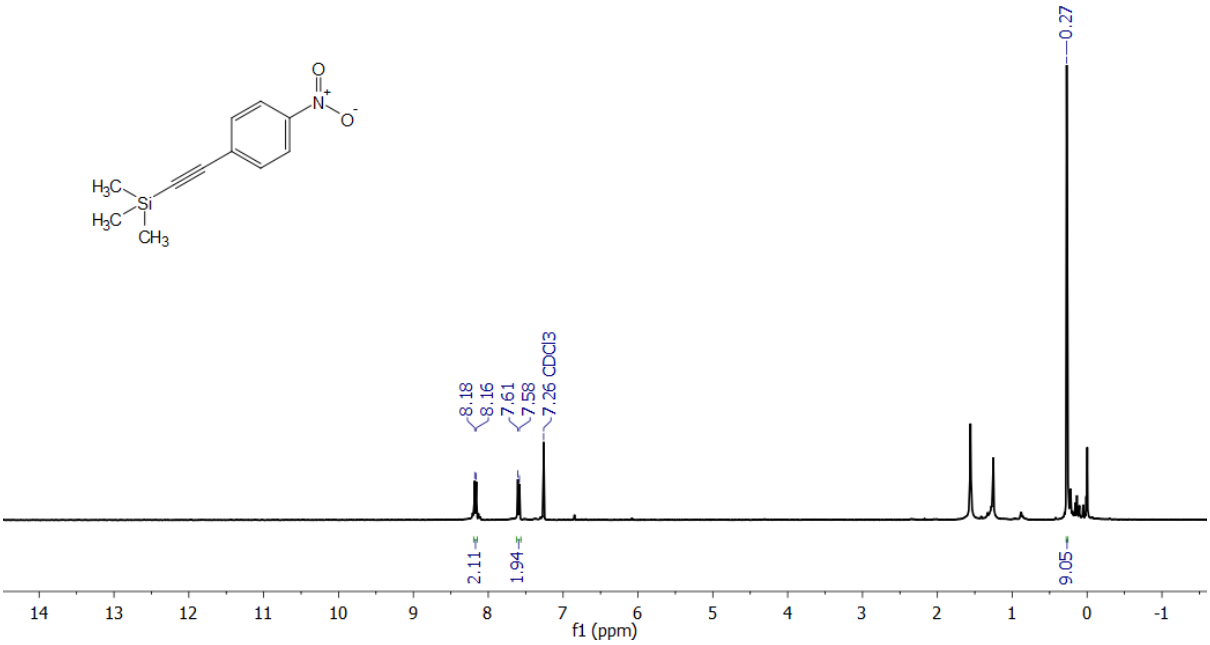
^{1}H NMR (400MHz, $CDCl_3$)



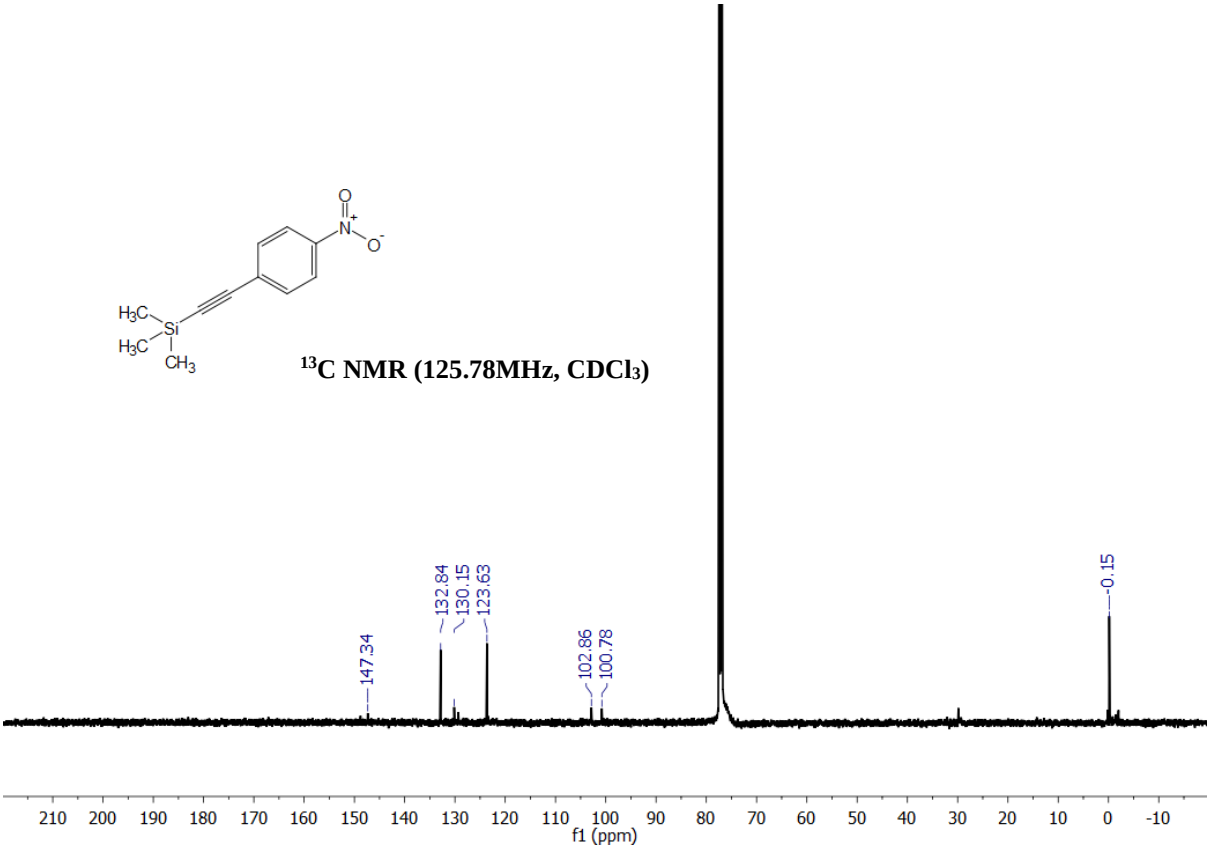
^{13}C NMR (125.78MHz, $CDCl_3$)

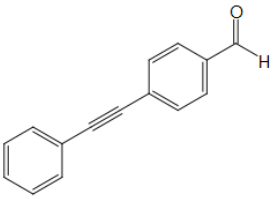


^{1}H NMR (400MHz, $CDCl_3$)

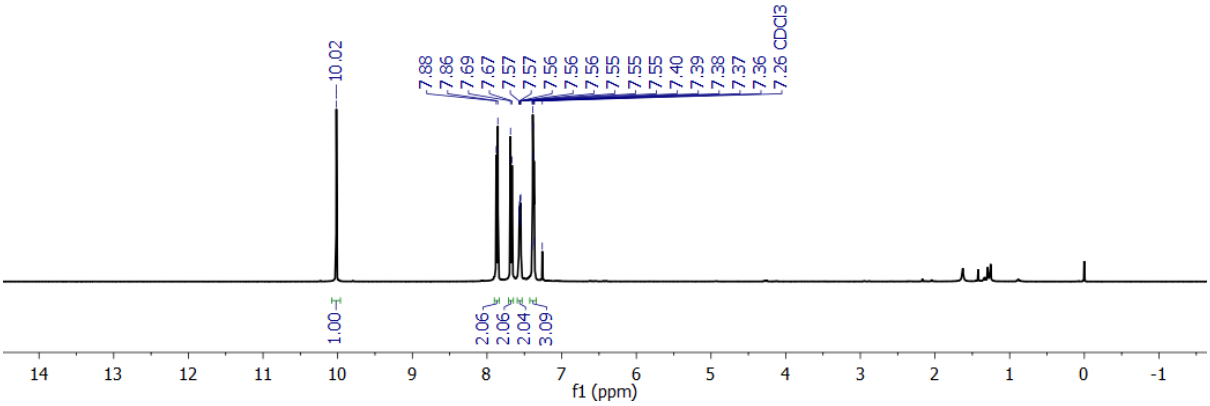


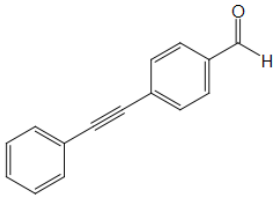
^{13}C NMR (125.78MHz, $CDCl_3$)



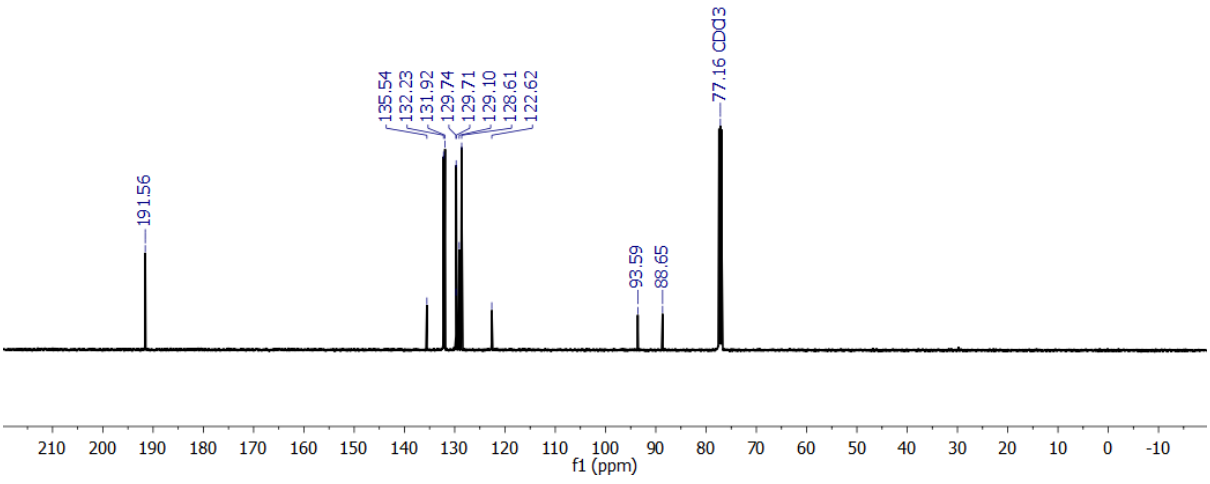


^{1}H NMR (400MHz, $CDCl_3$)

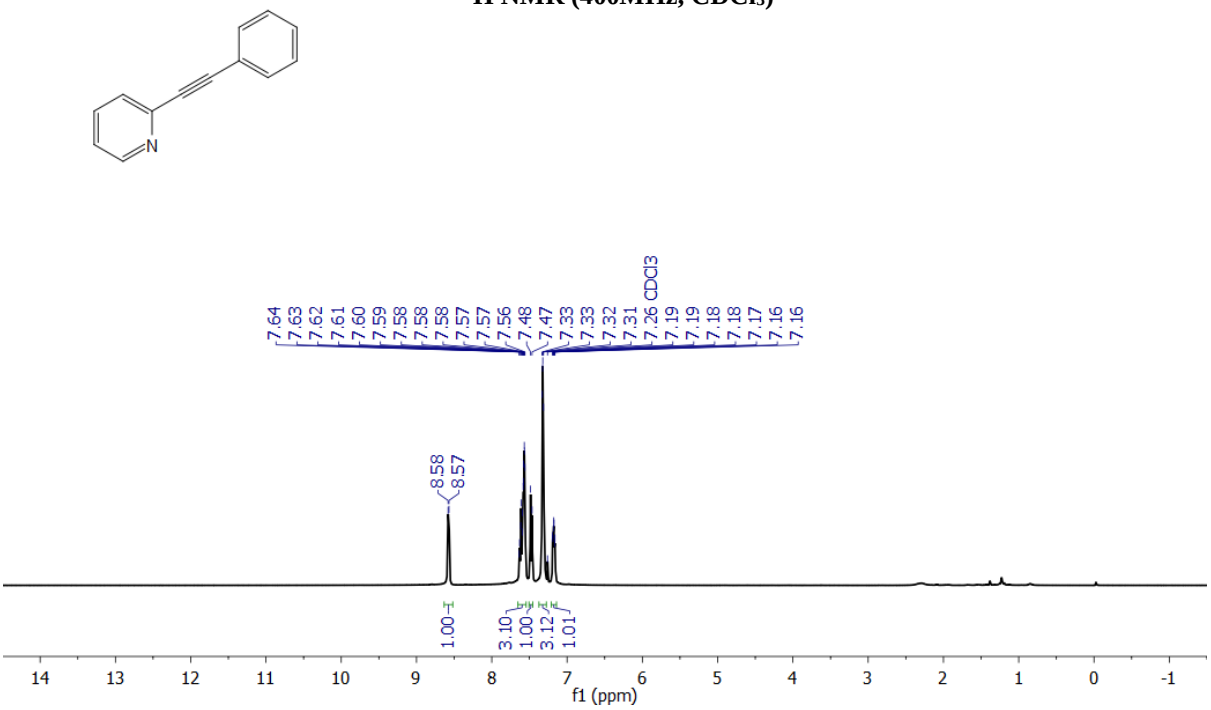




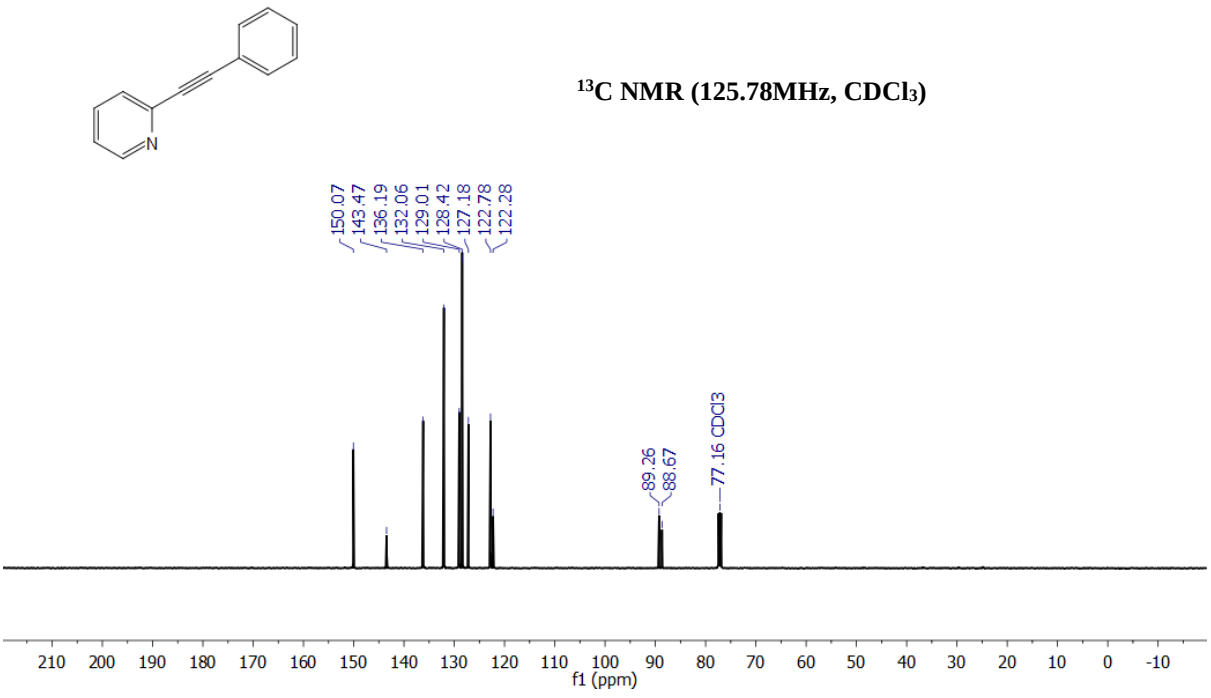
^{13}C NMR (125.78MHz, $CDCl_3$)



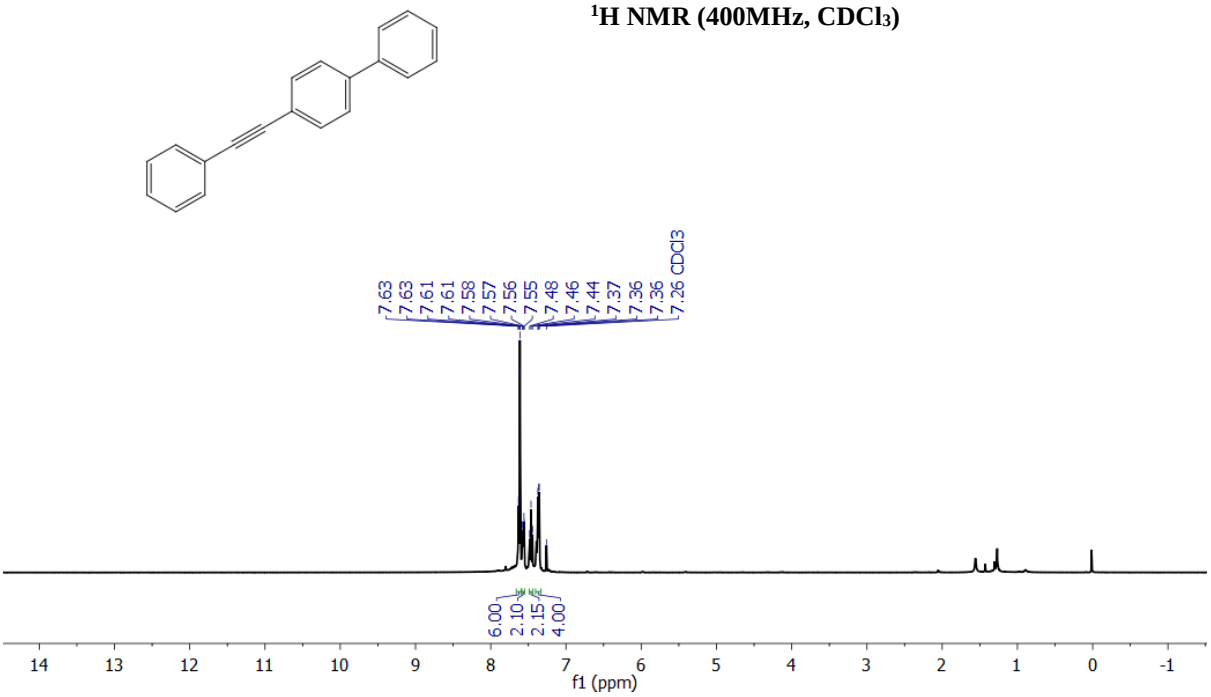
^{1}H NMR (400MHz, $CDCl_3$)



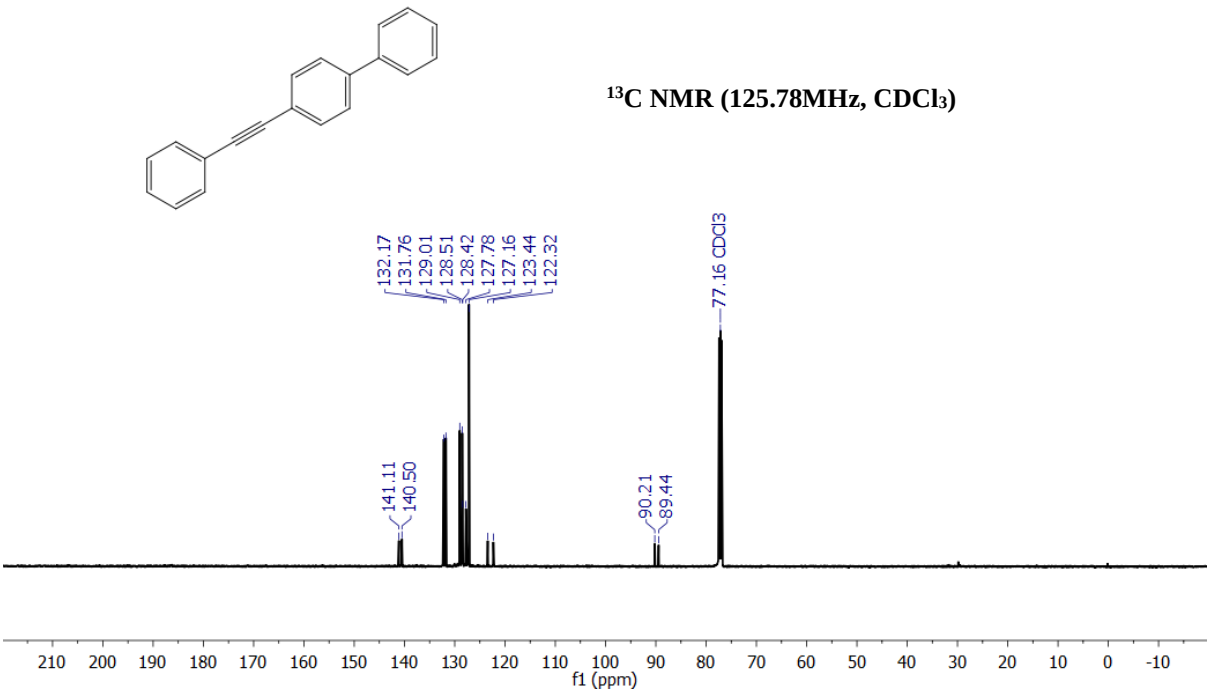
^{13}C NMR (125.78MHz, $CDCl_3$)



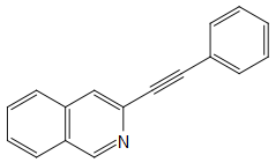
^{1}H NMR (400MHz, $CDCl_3$)

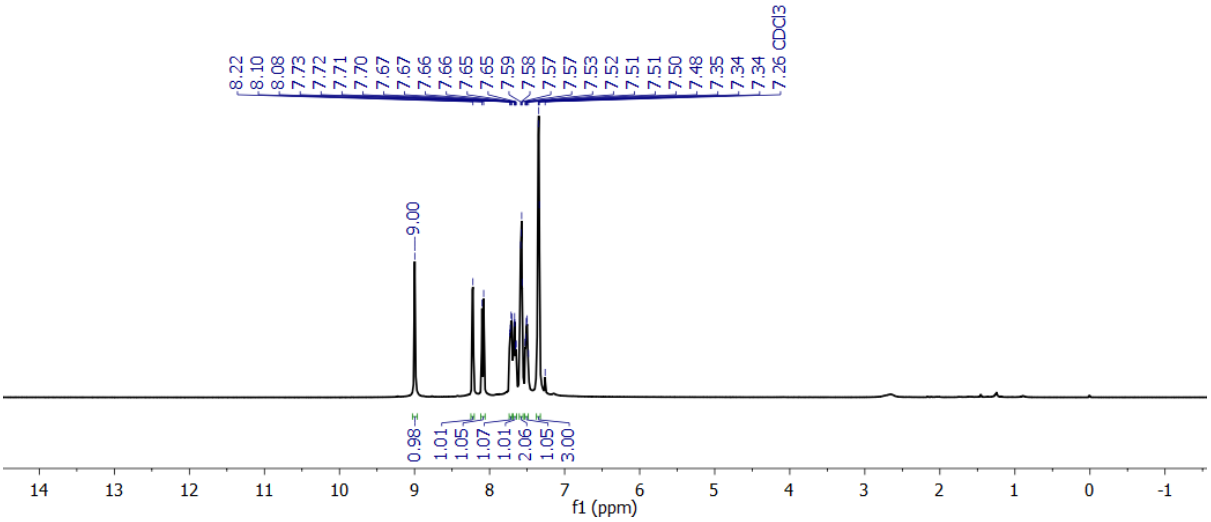


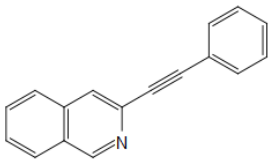
^{13}C NMR (125.78MHz, $CDCl_3$)



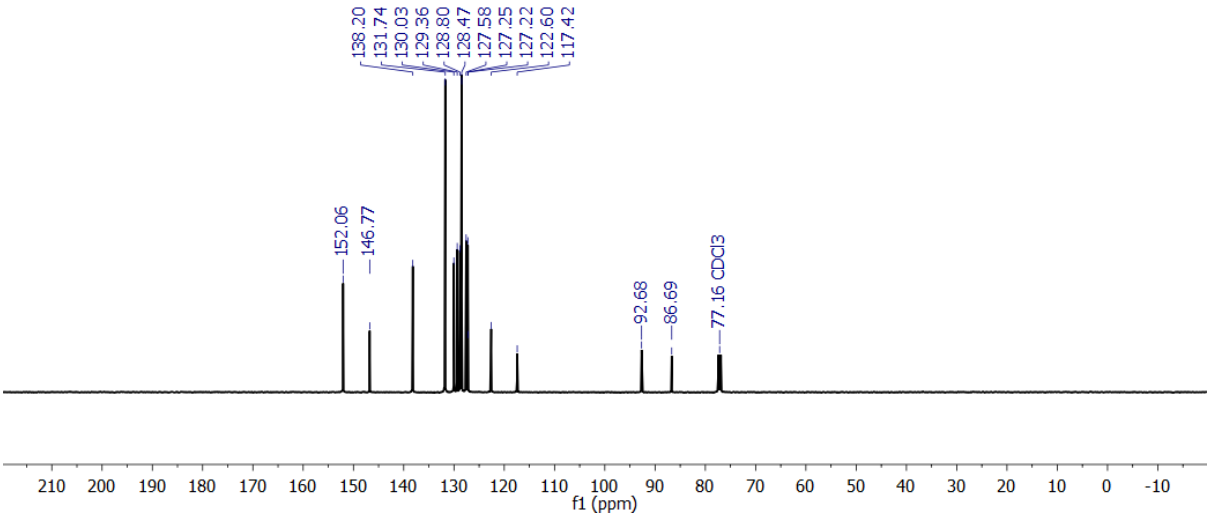
^{1}H NMR (400MHz, $CDCl_3$)



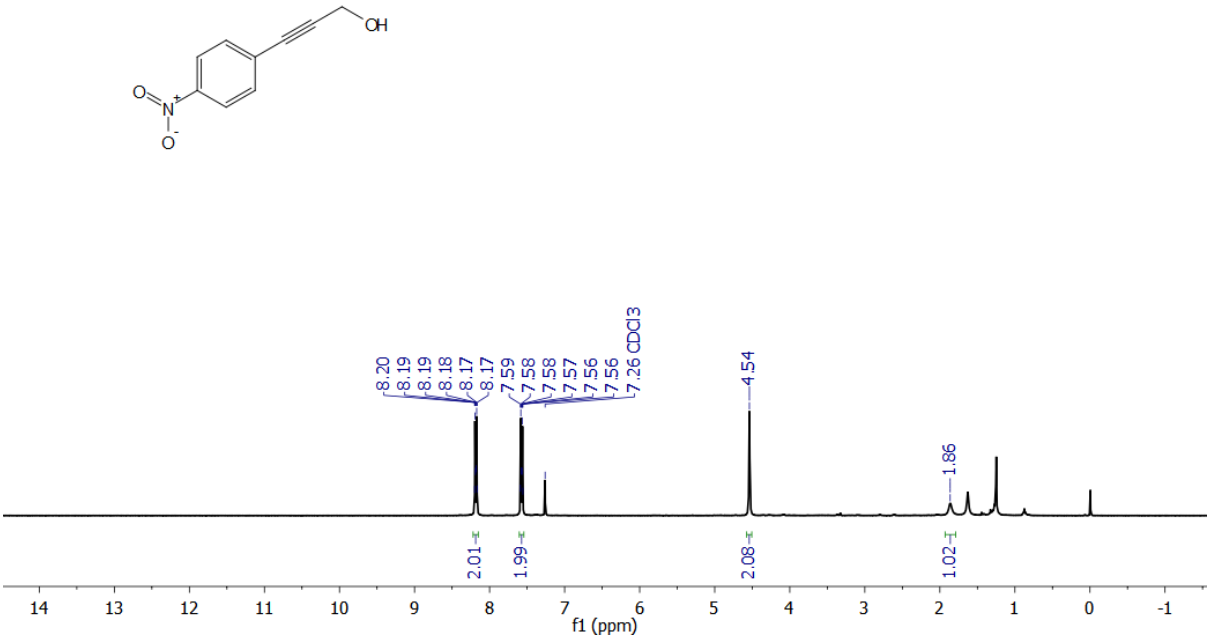




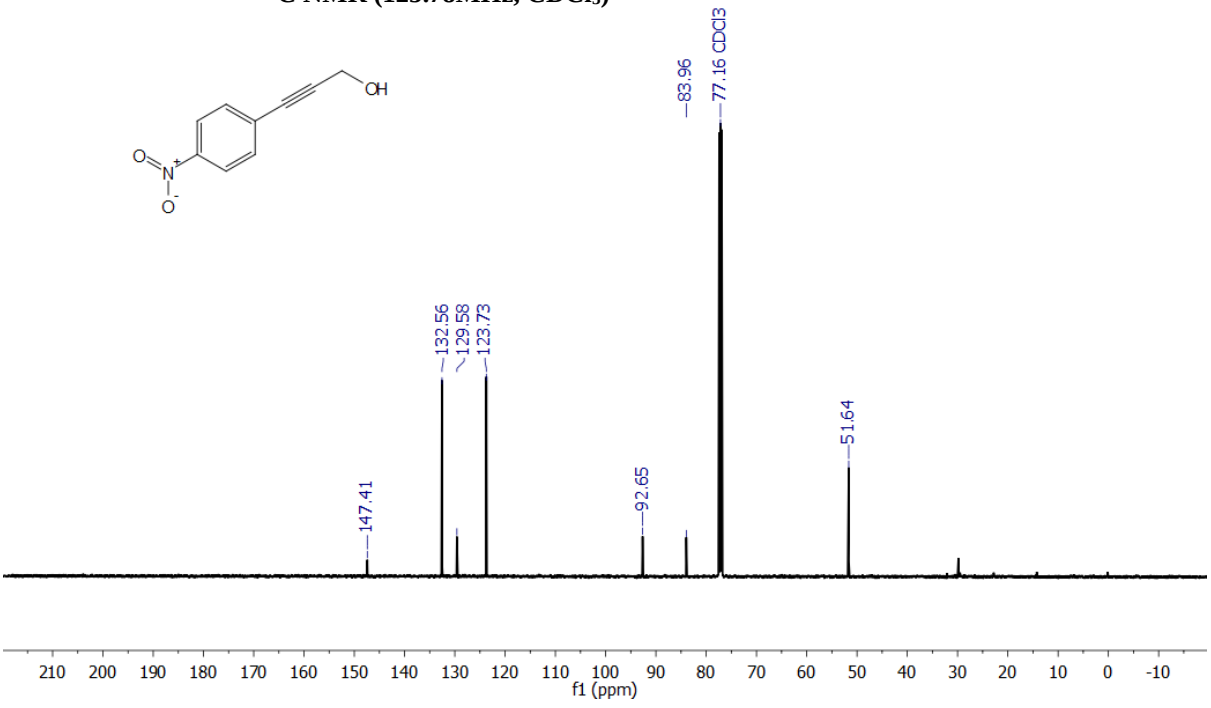
^{13}C NMR (125.78MHz, $CDCl_3$)



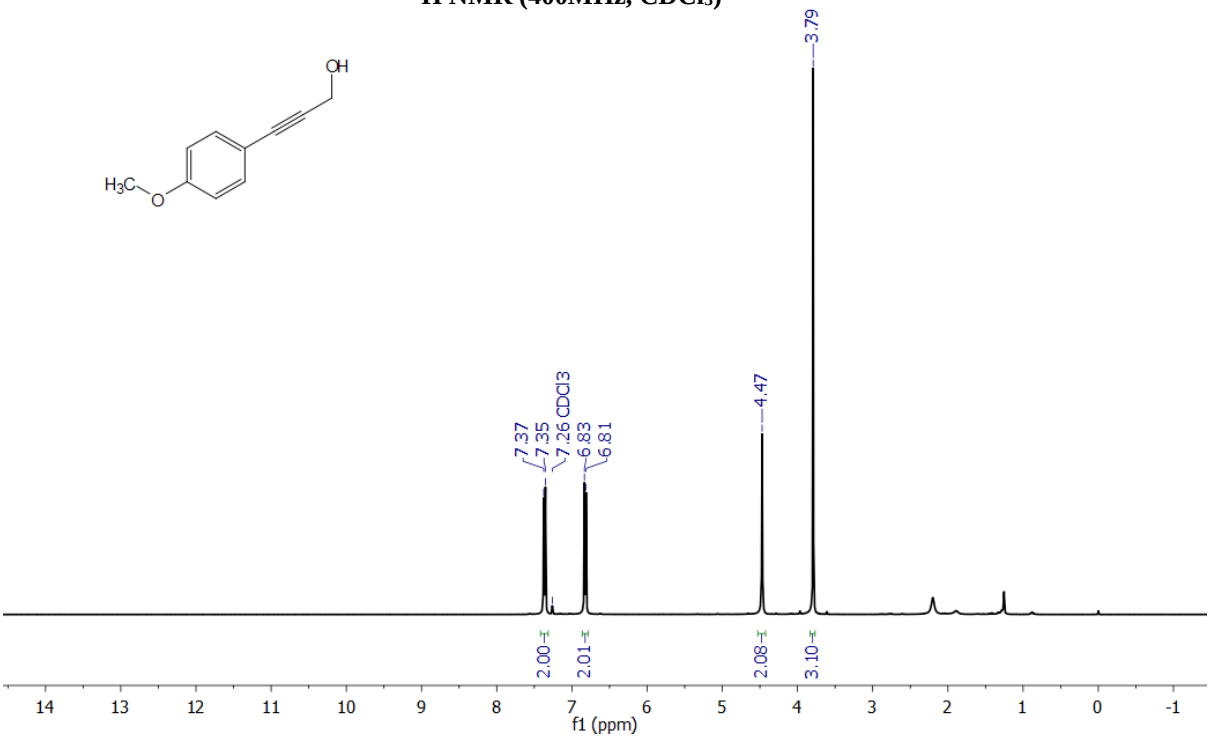
^{1}H NMR (400MHz, $CDCl_3$)



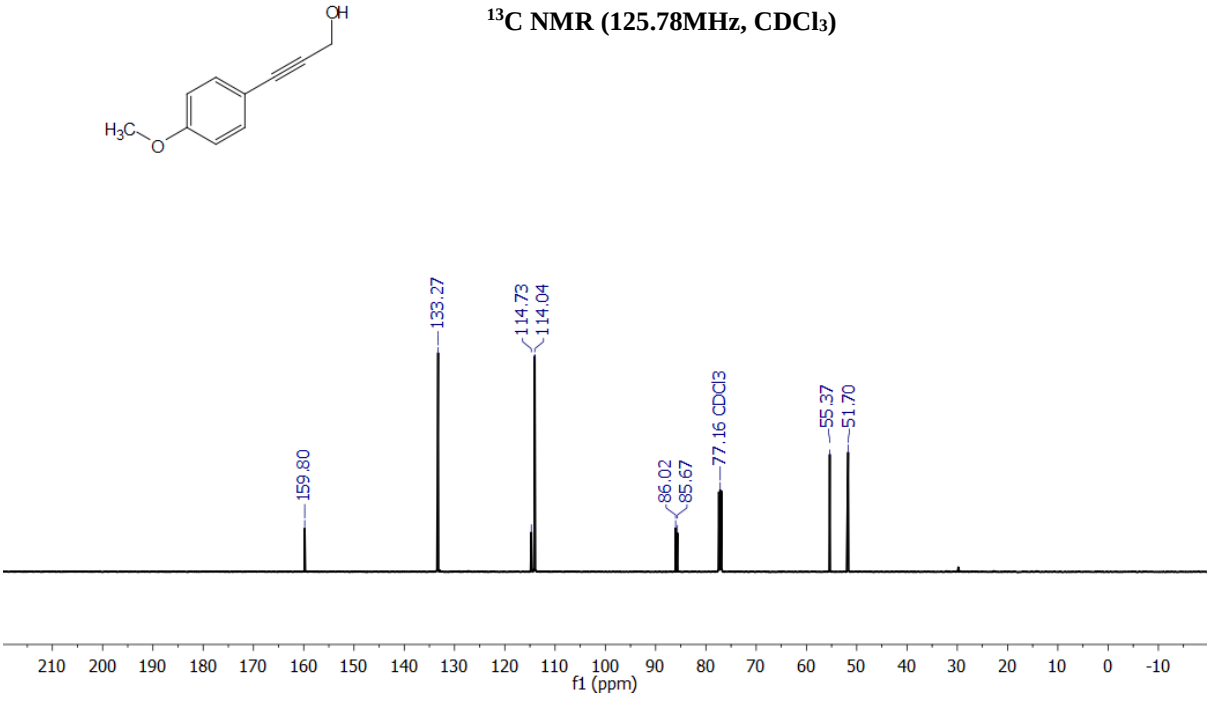
^{13}C NMR (125.78MHz, $CDCl_3$)

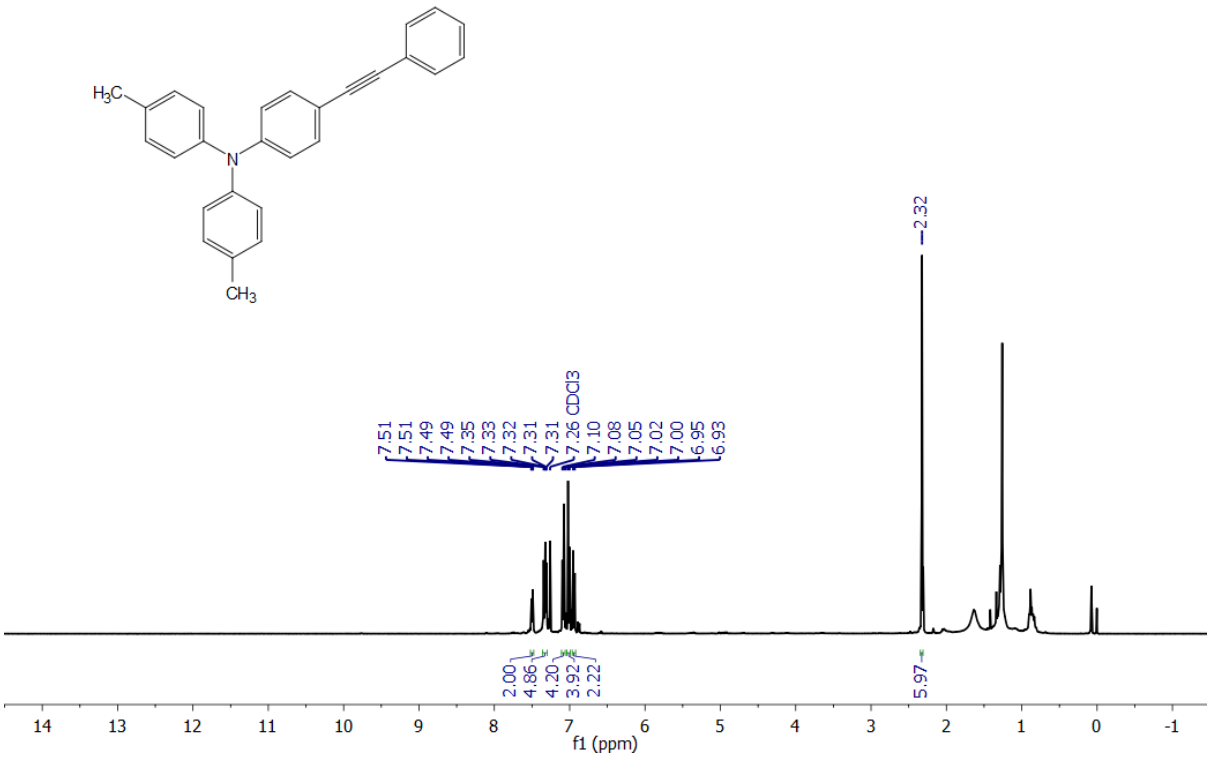


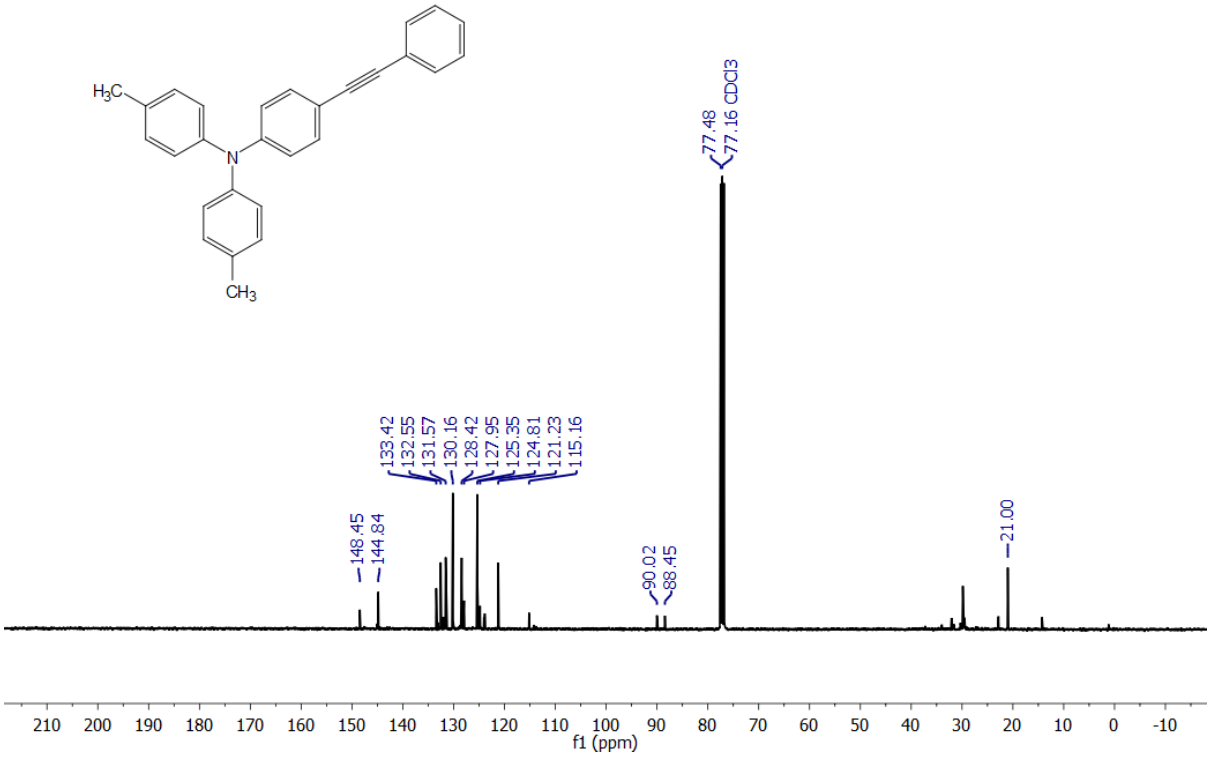
^{1}H NMR (400MHz, $CDCl_3$)

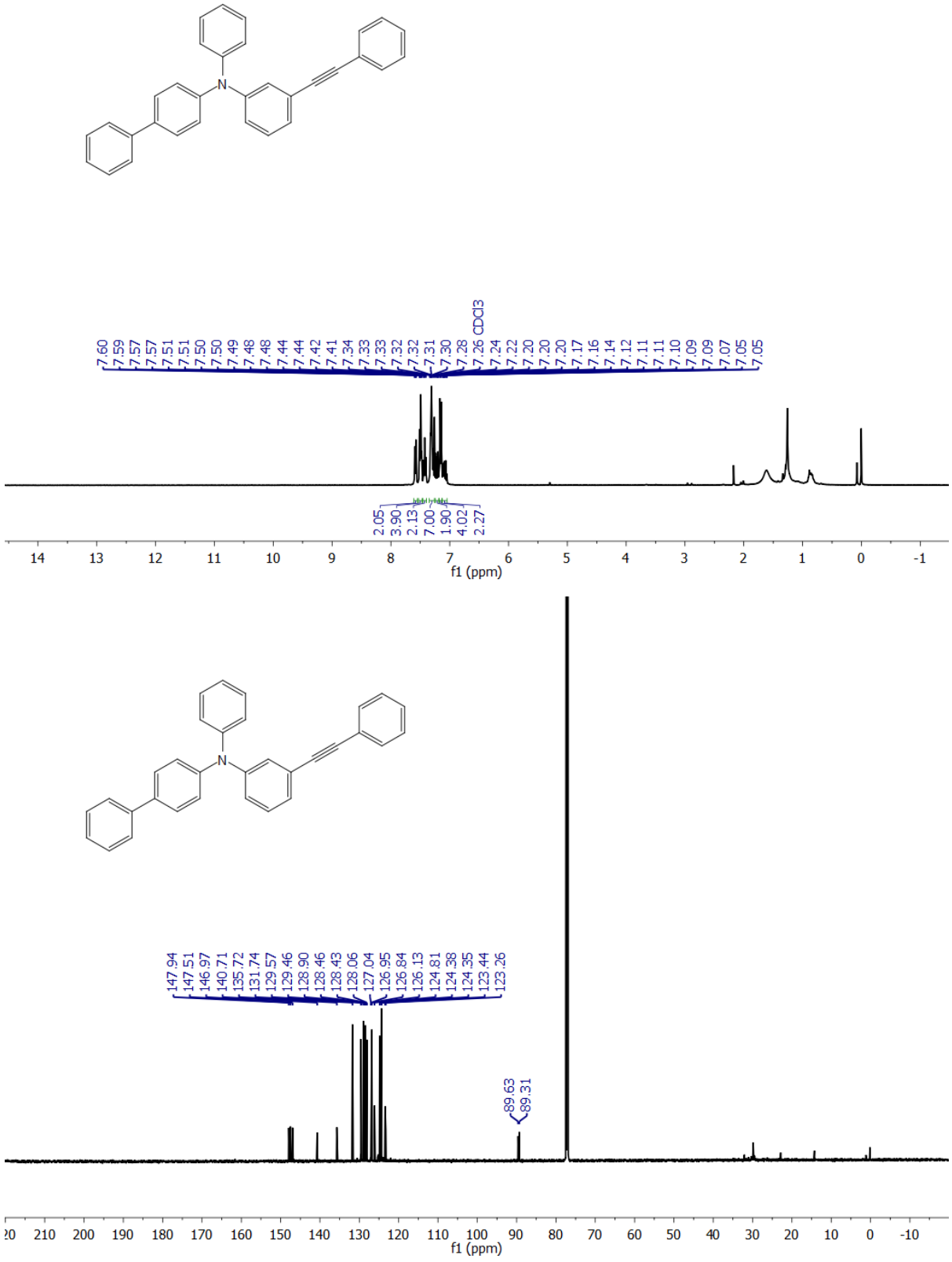


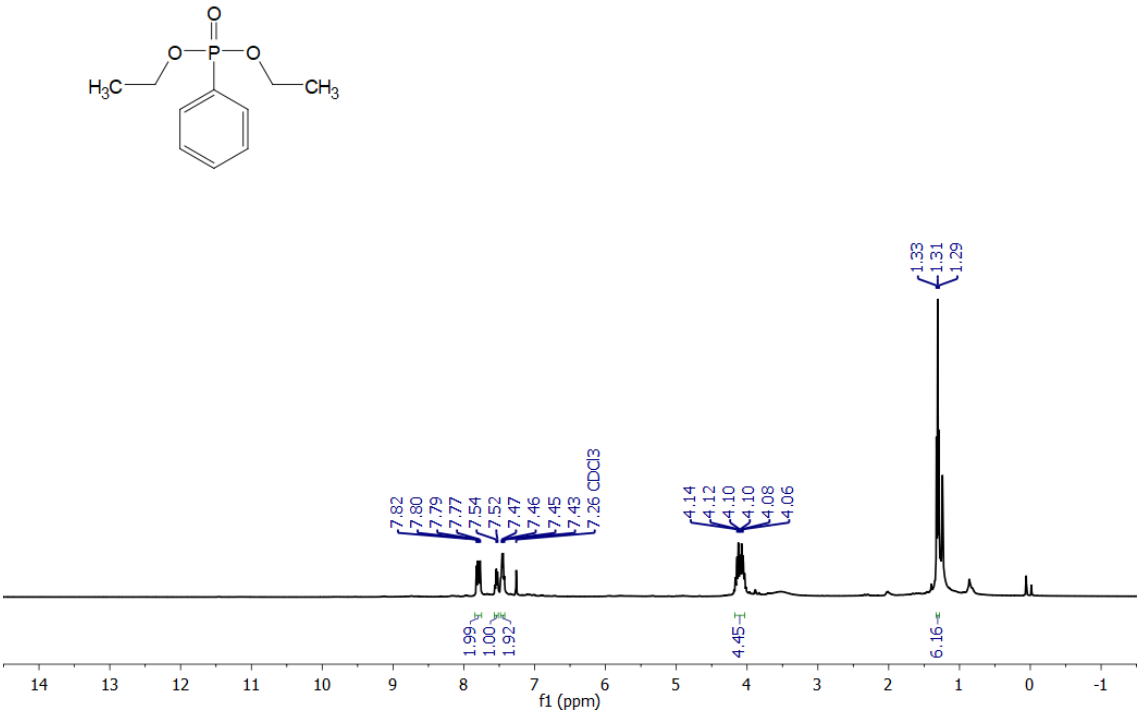
^{13}C NMR (125.78MHz, $CDCl_3$)

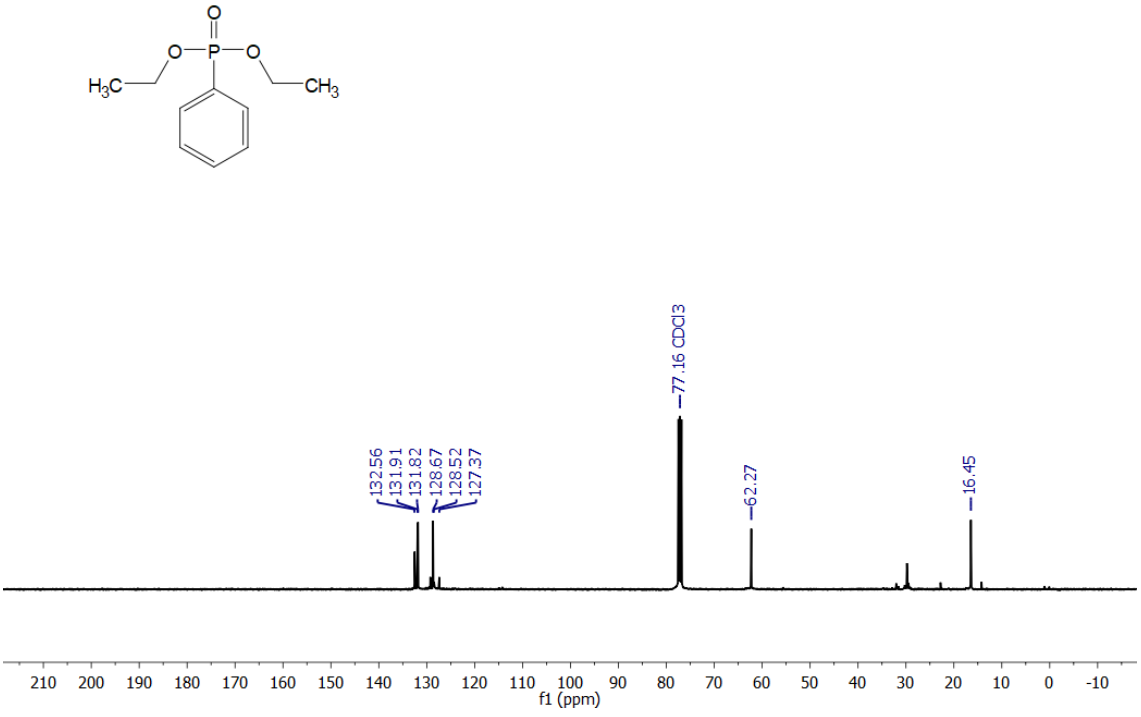


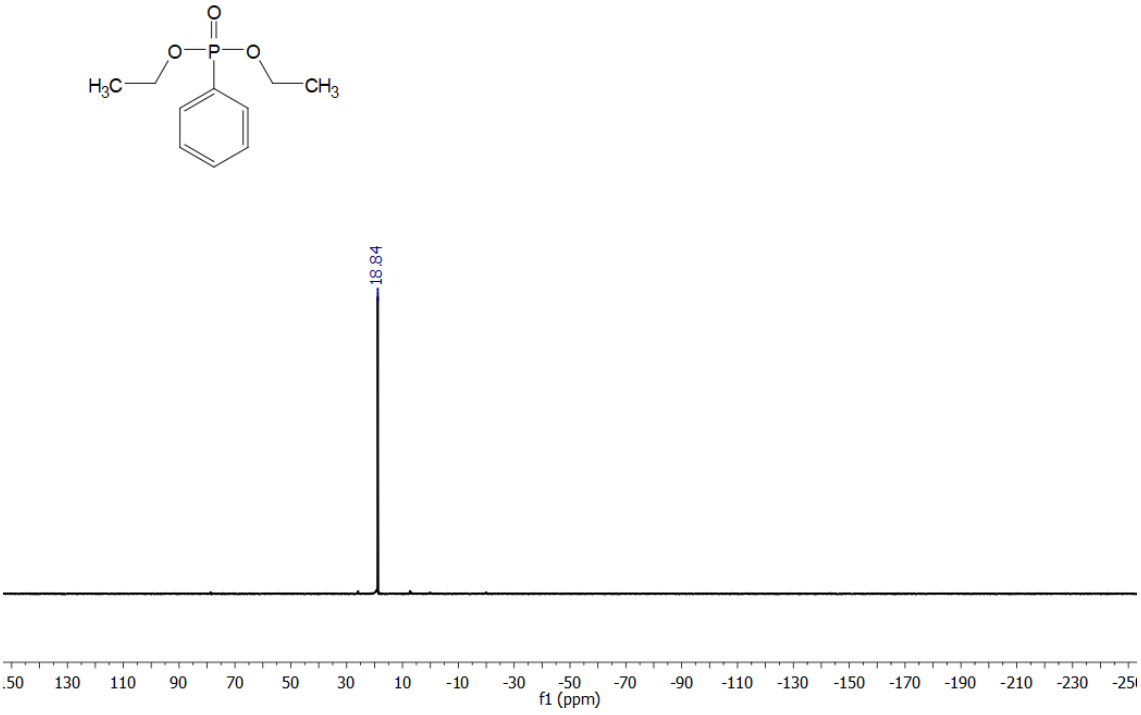

H3C
N
CH3
7.51
7.51
7.49
7.49
7.35
7.33
7.32
7.31
7.31
7.26 CDCl3
7.10
7.08
7.05
7.02
7.00
6.95
6.93
2.32
2.00
4.86
4.20
3.92
2.22
5.97
f1 (ppm)

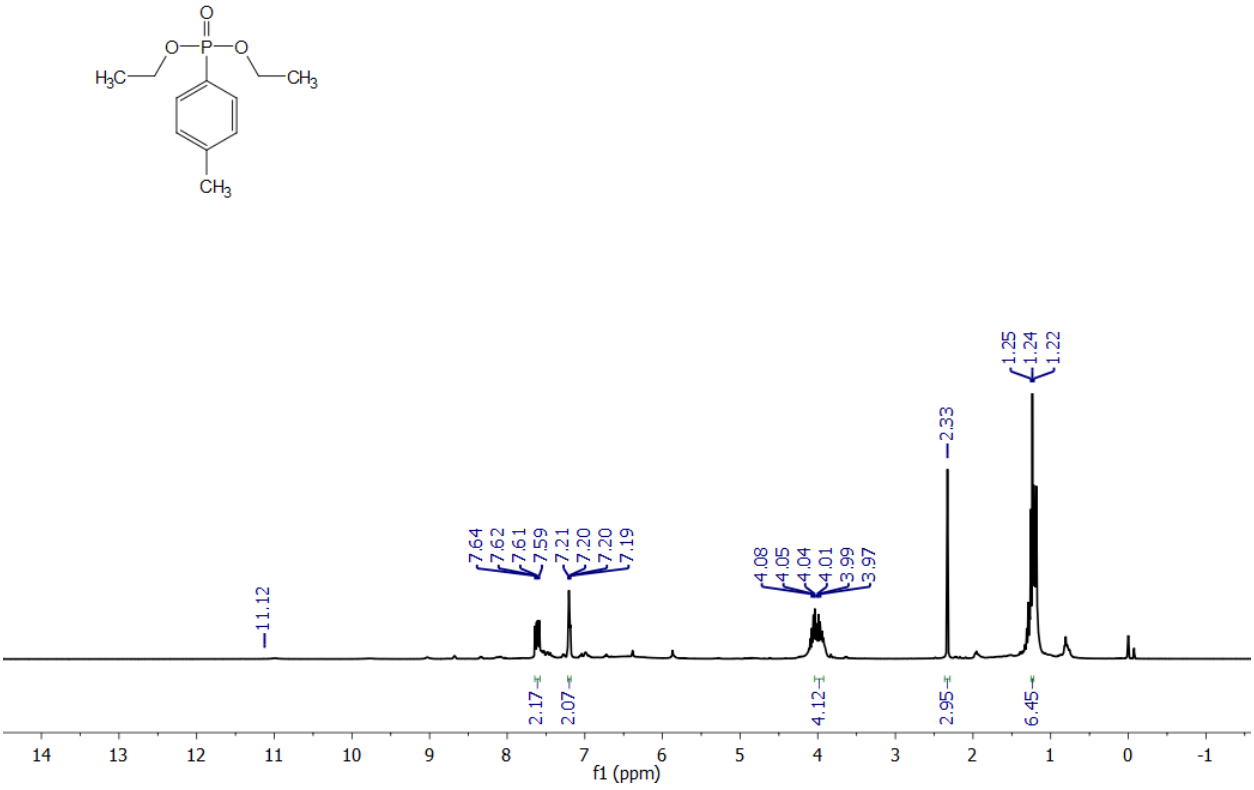

H3C
N
CH3
77.48
77.16 CDCl3
133.42
132.55
131.57
130.16
128.42
127.95
125.35
124.81
121.23
115.16
148.45
144.84
90.02
88.45
21.00
f1 (ppm)

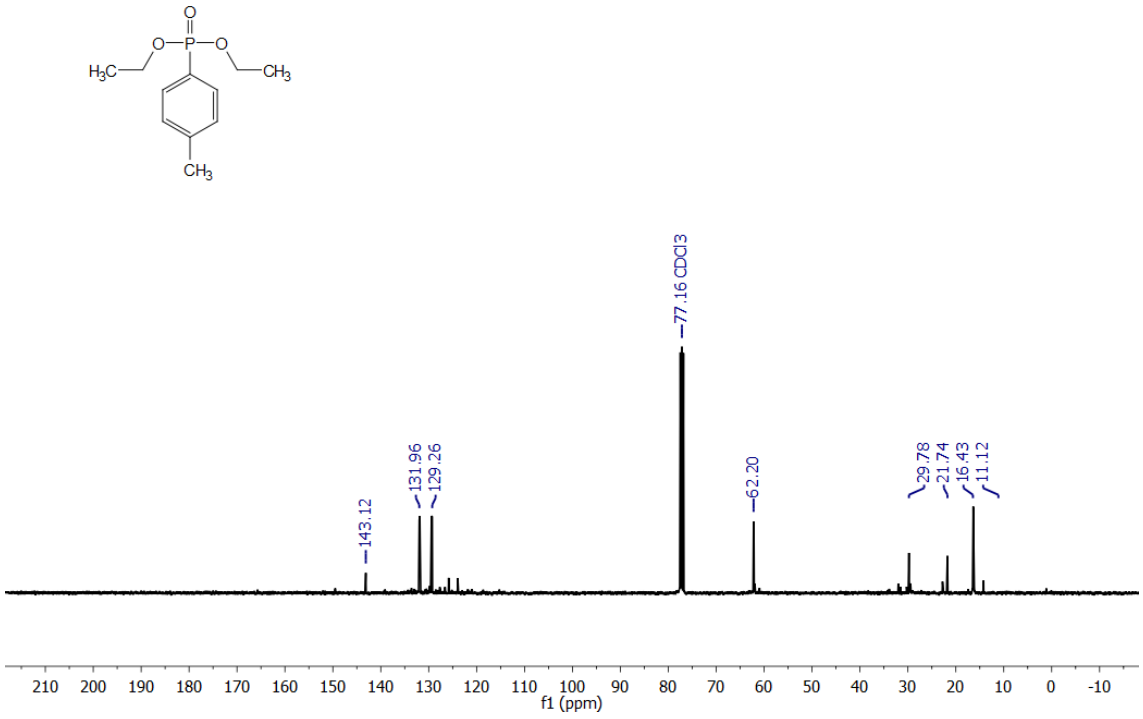

7.60
7.59
7.57
7.57
7.51
7.51
7.50
7.50
7.49
7.48
7.48
7.44
7.44
7.42
7.41
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.28
CDCl3
7.26
7.24
7.22
7.20
7.20
7.20
7.17
7.16
7.14
7.12
7.11
7.11
7.10
7.09
7.09
7.07
7.05
7.05
2.05
3.90
2.13
7.00
1.90
4.02
2.27
f1 (ppm)
147.94
147.51
146.97
140.71
135.72
131.74
129.57
129.46
128.90
128.46
128.43
128.06
127.04
126.95
126.84
126.13
124.81
124.38
124.35
123.44
123.26
89.63
89.31
f1 (ppm)

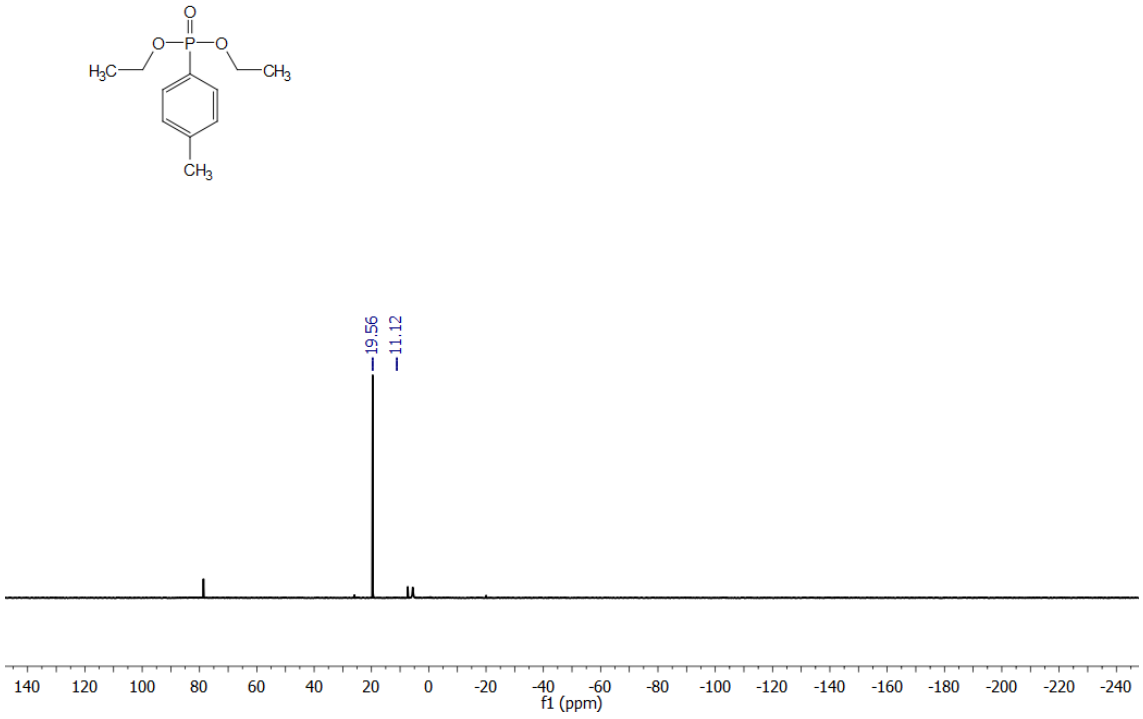

O
O
P
O
H3C
CH3
7.82
7.80
7.79
7.77
7.54
7.52
7.47
7.46
7.45
7.43
7.26 CDCl3
4.14
4.12
4.10
4.10
4.08
4.06
1.33
1.31
1.29
1.99
1.00
1.92
4.45
6.16
f1 (ppm)

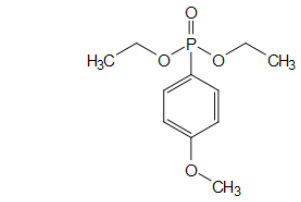

O
O
P
O
H3C
CH3
132.56
131.91
131.82
128.67
128.52
127.37
77.16 CDCl3
62.27
16.45
f1 (ppm)

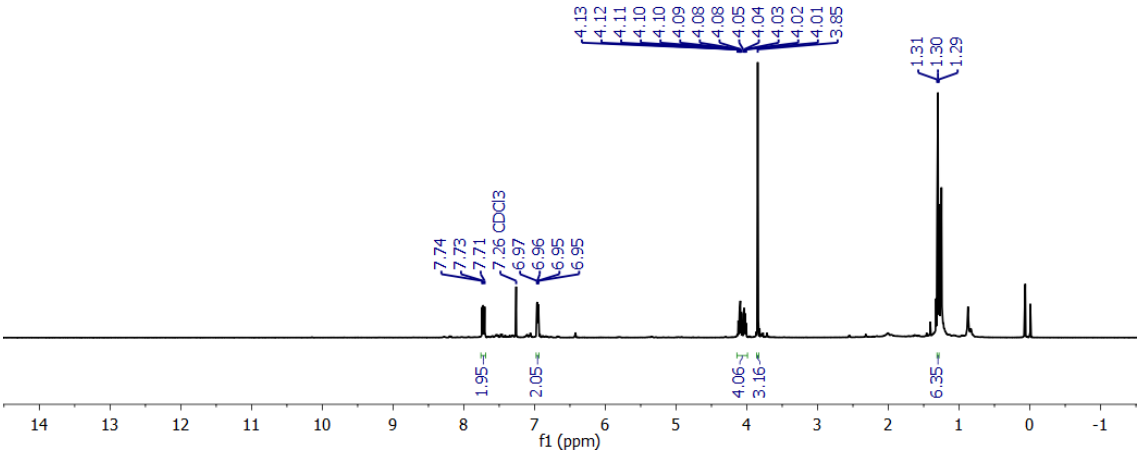

O
O
P
O
H3C
CH3
18.84
f1 (ppm)

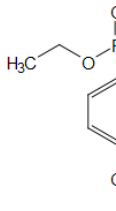

O
O
P
O
H3C
CH3
CH3
11.12
7.64
7.62
7.61
7.59
7.21
7.20
7.20
7.19
4.08
4.05
4.04
4.01
3.99
3.97
2.33
1.25
1.24
1.22
2.17
2.07
4.12
2.95
6.45
f1 (ppm)


143.12
131.96
129.26
77.16 CDCl3
62.20
29.78
21.74
16.43
11.12
f1 (ppm)

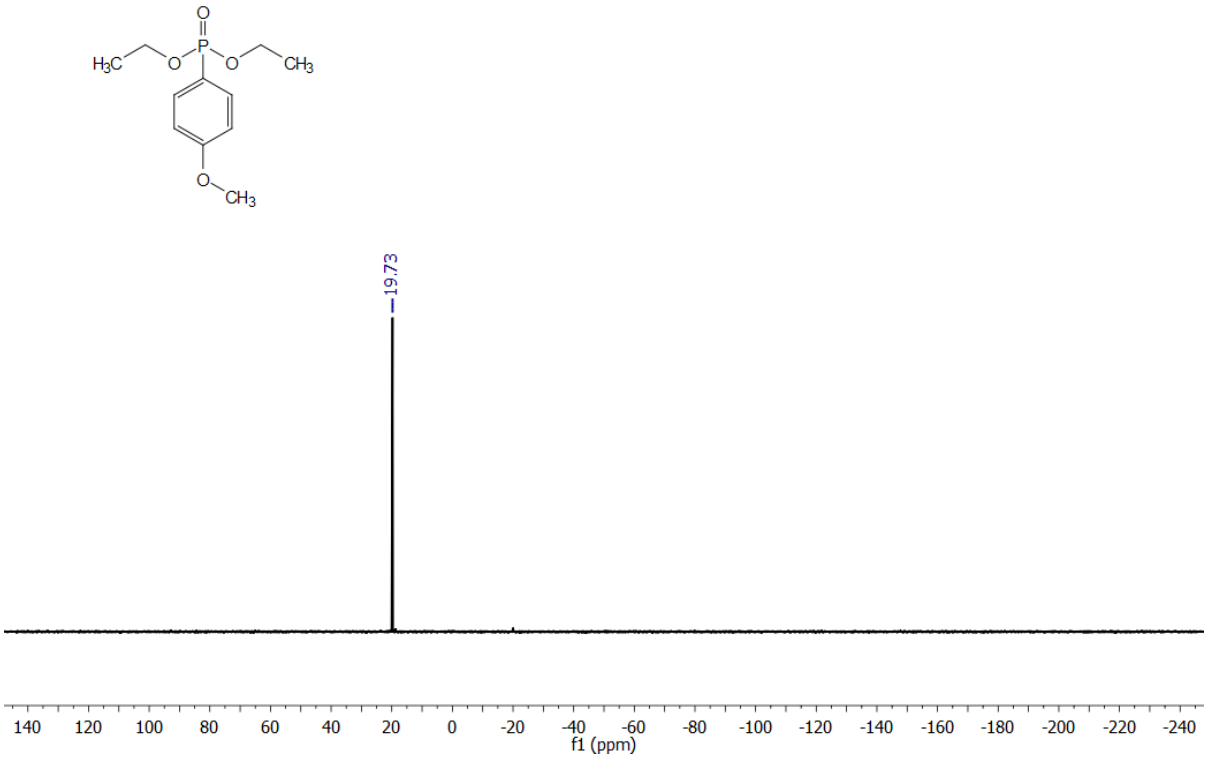

19.56
11.12
f1 (ppm)

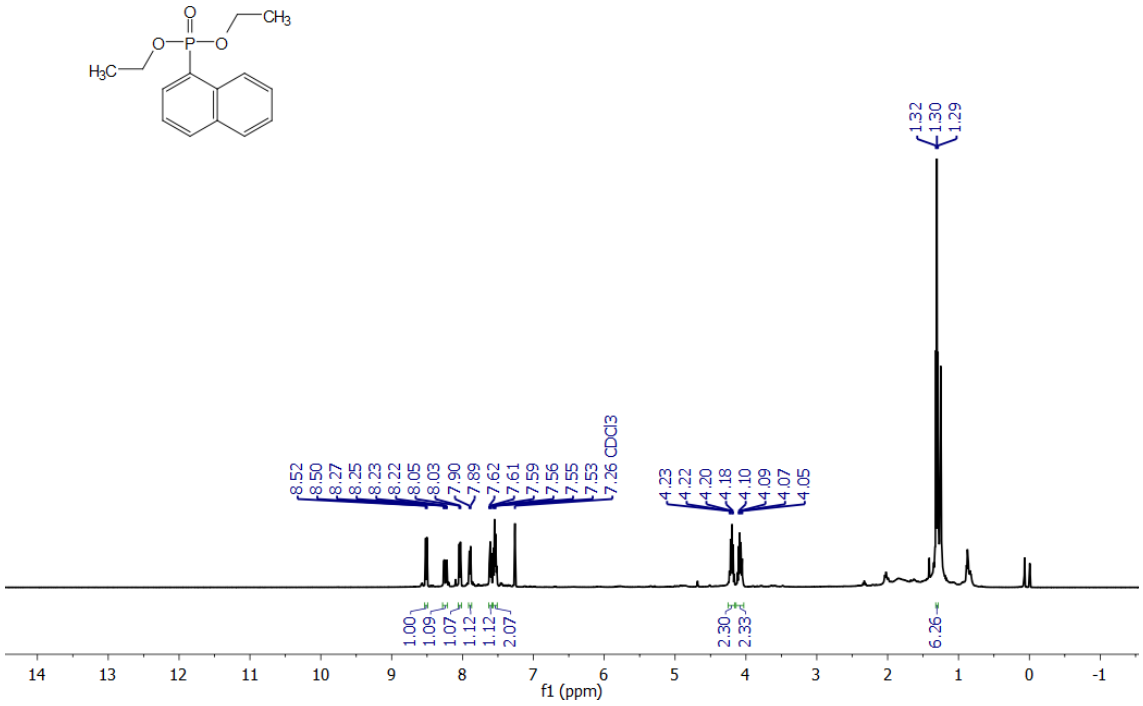

O
P
H3C
O
O
CH3
O
CH3

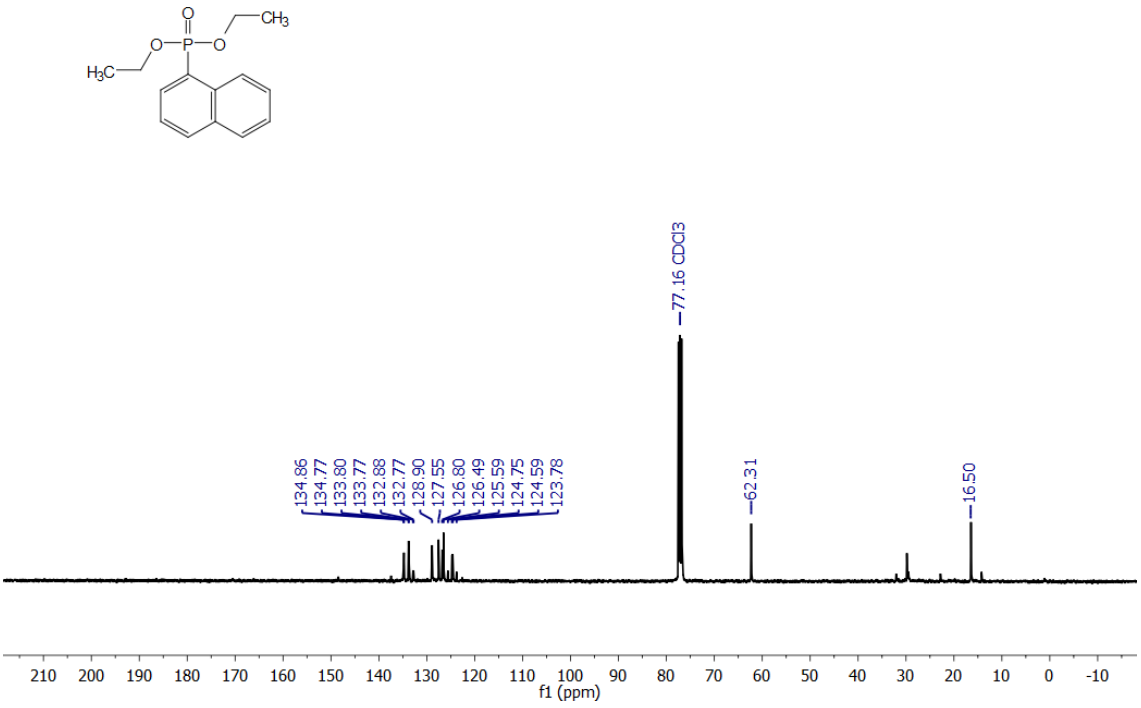

4.13
4.12
4.11
4.10
4.10
4.09
4.08
4.08
4.05
4.04
4.03
4.02
4.01
3.85
1.31
1.30
1.29
7.74
7.73
7.71
7.26 CDCl3
6.97
6.96
6.95
6.95
1.95
2.05
4.06
3.16
6.35
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

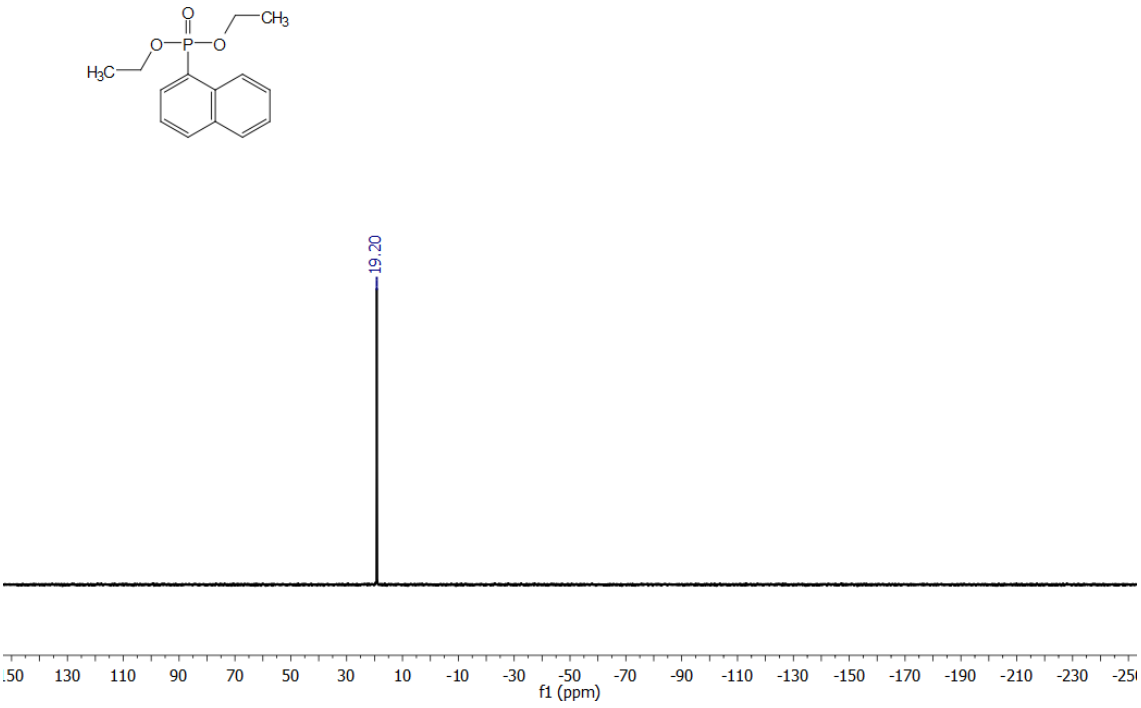

O
P
H3C
O
O
CH3
O
CH3

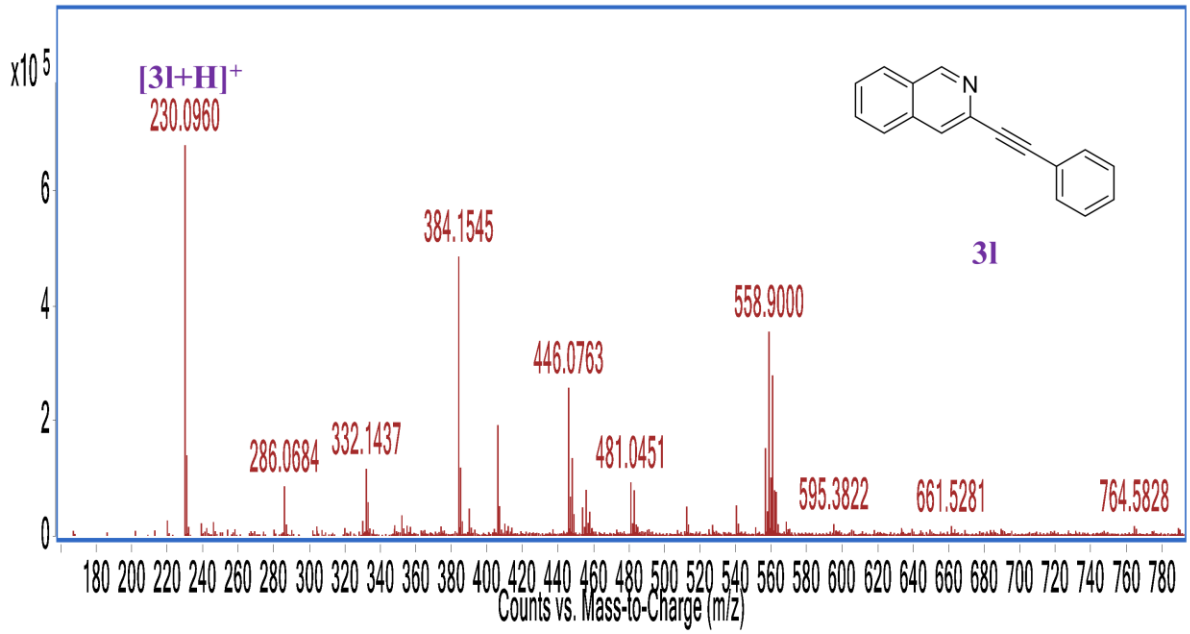
77.16 CDCl3
162.99
133.93
133.86
118.89
114.22
114.11
62.12
62.08
55.48
16.47
16.42
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

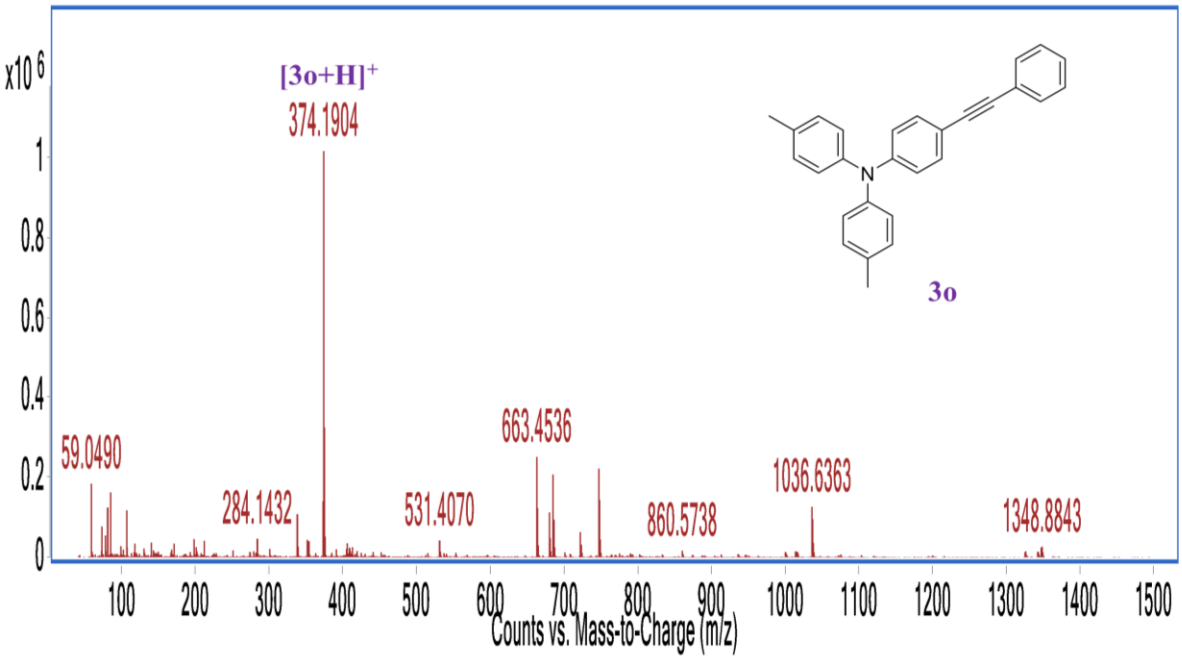

19.73
140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240
f1 (ppm)


8.52
8.50
8.27
8.25
8.23
8.22
8.05
8.03
7.90
7.89
7.62
7.61
7.59
7.56
7.55
7.53
7.26 CDCl3
4.23
4.22
4.20
4.18
4.10
4.09
4.07
4.05
1.32
1.30
1.29
1.00
1.09
1.07
1.12
1.12
2.07
2.30
2.33
6.26
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


O
CH3
O
P
O
H3C
77.16 CDCl3
134.86
134.77
133.80
133.77
132.88
132.77
128.90
127.55
126.80
126.49
125.59
124.75
124.59
123.78
62.31
16.50
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
CH3
O
P
O
H3C
19.20
50 130 110 90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)


x10 5
[3l+H]+
230.0960
384.1545
558.9000
446.0763
286.0684
332.1437
481.0451
595.3822
661.5281
764.5828
N
3l
Counts vs. Mass-to-Charge (m/z)


x10 6
[3o+H]+
374.1904
663.4536
59.0490
1036.6363
284.1432
531.4070
860.5738
1348.8843
N
3o
Counts vs. Mass-to-Charge (m/z)

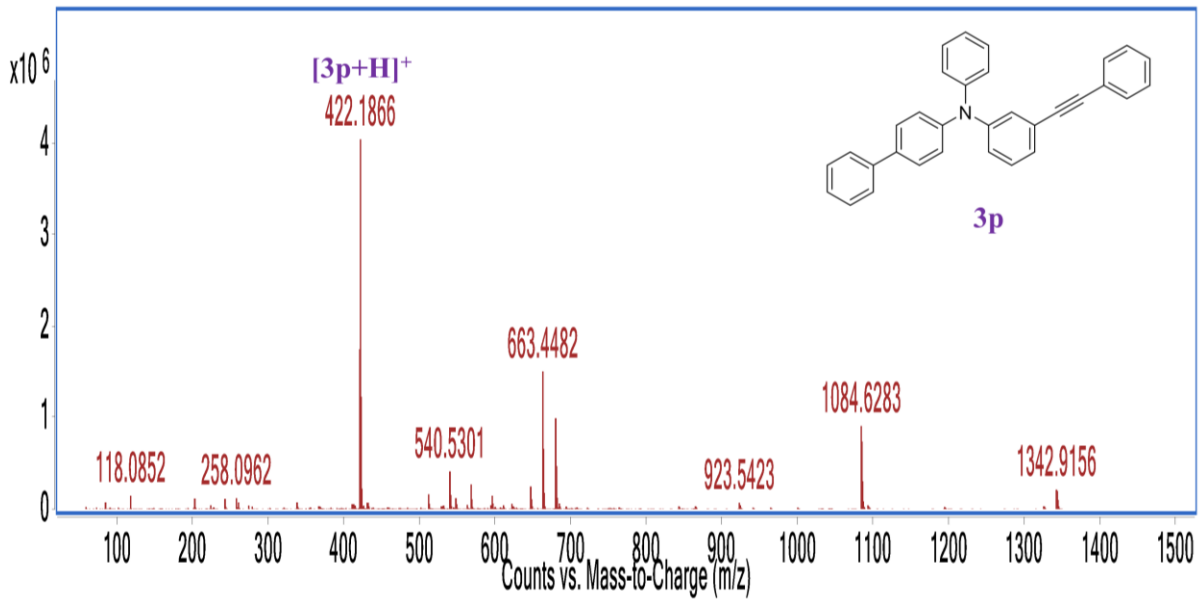


Figure S32. HRMS (ESI) spectrum of **3l**, **3o** and **3p**.

Table S25: Crystallographic data and refinement parameters of **3o**

Identification code	**3o**
Empirical formula	$C_{28}H_{23}N$
Formula weight	373.47
Temperature/K	297.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.992(5)
b/Å	12.228(6)
c/Å	17.586(9)
α/°	90
β/°	97.053(15)
γ/°	90
Volume/Å^3	2132.6(19)
Z	4
ρ_{calc}g/cm^3	1.163
μ/mm^{-1}	0.067

F(000)	792.0
Crystal size/mm^3	0.2 × 0.17 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.068 to 54.516
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 15, -22 ≤ l ≤ 22
Reflections collected	56226
Independent reflections	4658 [R_{int} = 0.0680, R_{sigma} = 0.0471]
Data/restraints/parameters	4658/225/264
Goodness-of-fit on F^2	1.153
Final R indexes [I>=2σ (I)]	R_1 = 0.0997, wR_2 = 0.2084
Final R indexes [all data]	R_1 = 0.1681, wR_2 = 0.2461
Largest diff. peak/hole / e Å^{-3}	0.32/-0.18

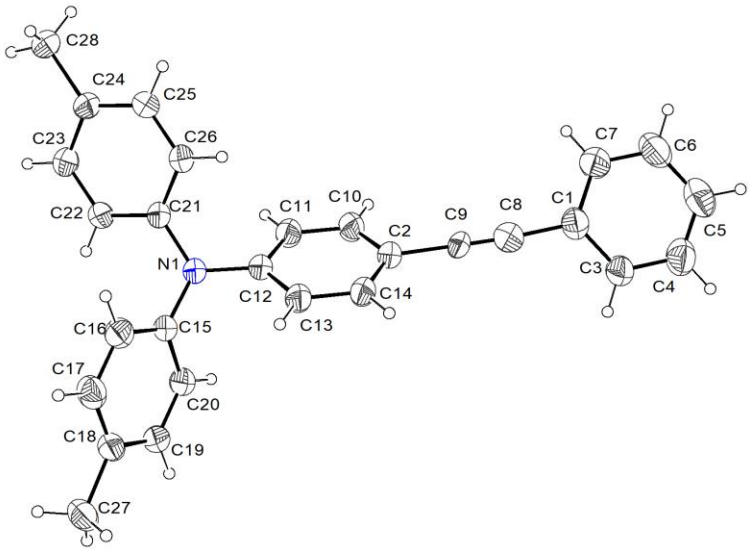


Figure S33: ORTEP diagram of **5**. Thermal ellipsoids are drawn at 30% probability level and solvents molecules were omitted for clarity.

Table S26: Bond lengths in **3o**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C12	1.420(4)	C12	C13	1.392(5)	C17	C18	1.380(5)
N1	C15	1.420(4)	C13	C14	1.376(5)	C18	C19	1.372(5)
N1	C21	1.428(4)	C15	C16	1.385(5)	C18	C27	1.551(5)

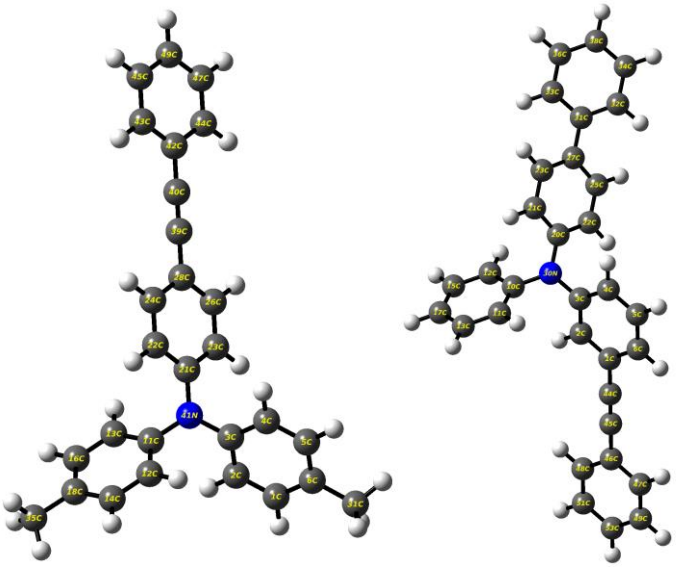
C1	C3	1.397(6)	C15	C20	1.374(5)	C19	C20	1.378(5)
C1	C7	1.395(5)	C16	C17	1.381(5)	C21	C22	1.381(5)
C1	C8	1.477(6)	C4	C5	1.369(7)	C21	C26	1.381(5)
C2	C9	1.517(5)	C5	C6	1.407(7)	C22	C23	1.382(5)
C2	C10	1.384(5)	C6	C7	1.343(6)	C23	C24	1.379(5)
C2	C14	1.384(5)	C8	C9	1.091(5)	C24	C25	1.373(5)
C3	C4	1.360(6)	C10	C11	1.384(5)	C24	C28	1.583(5)
C11	C12	1.385(5)	C25	C26	1.378(5)			

Table S27: Bond angles in **3o**

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	N1	C15	119.2(3)	C13	C14	C2	121.2(3)
C12	N1	C21	119.3(3)	C16	C15	N1	122.5(3)
C15	N1	C21	119.8(2)	C20	C15	N1	119.7(3)
C3	C1	C8	121.2(4)	C20	C15	C16	117.7(3)
C7	C1	C3	118.3(4)	C17	C16	C15	120.6(3)
C7	C1	C8	120.5(4)	C18	C17	C16	121.6(3)
C10	C2	C9	119.3(3)	C17	C18	C27	122.2(4)
C10	C2	C14	118.5(3)	C19	C18	C17	117.1(3)
C14	C2	C9	122.2(3)	C19	C18	C27	120.7(4)
C4	C3	C1	120.4(4)	C18	C19	C20	121.8(3)
C3	C4	C5	121.4(5)	C15	C20	C19	121.1(3)
C4	C5	C6	118.1(4)	C22	C21	N1	120.8(3)
C7	C6	C5	121.0(5)	C22	C21	C26	117.9(3)
C6	C7	C1	120.7(4)	C26	C21	N1	121.3(3)
C9	C8	C1	176.9(4)	C21	C22	C23	120.5(3)
C8	C9	C2	179.1(4)	C24	C23	C22	121.7(3)
C2	C10	C11	120.7(3)	C23	C24	C28	122.1(3)
C10	C11	C12	120.6(3)	C25	C24	C23	117.2(3)
C11	C12	N1	120.1(3)	C25	C24	C28	120.7(3)
C11	C12	C13	118.6(3)	C24	C25	C26	121.7(3)
C13	C12	N1	121.2(3)	C25	C26	C21	120.8(3)
C14	C13	C12	120.2(3)				

Computational study:

All calculations were performed by using Gaussian16 (G16) program[19] and the geometry of all ligands and complexes was optimized using B3LYP hybrid functional and 6-311g(d,p)/LanL2DZ basis set. Density functional theory (DFT) was used to model the frontier molecular orbitals to predict the kinetic stability and chemical reactivity. All computations such as optimized structure, contour plots of the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO) were visualized using GaussView 5.0.[20]



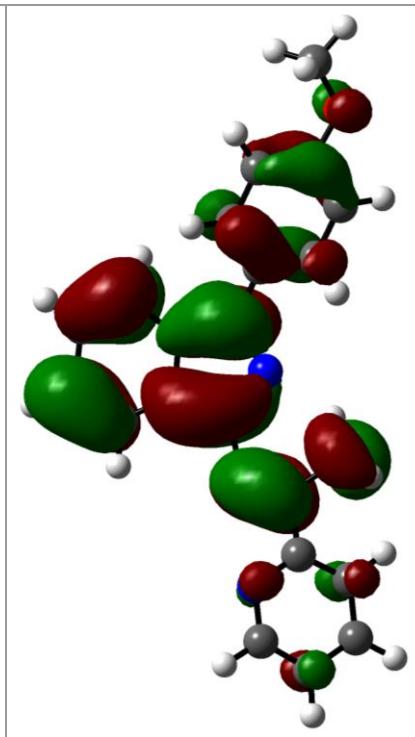
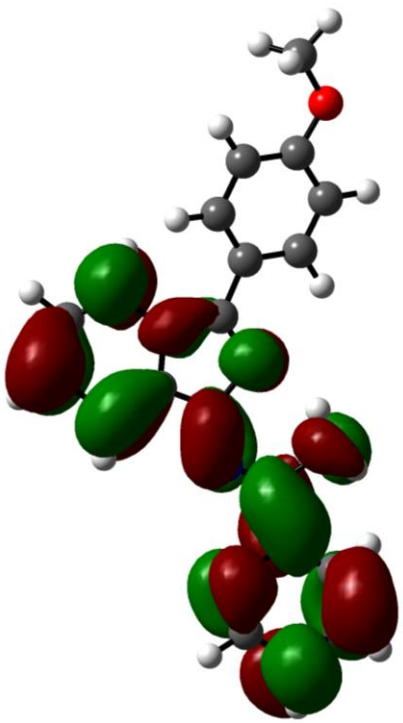
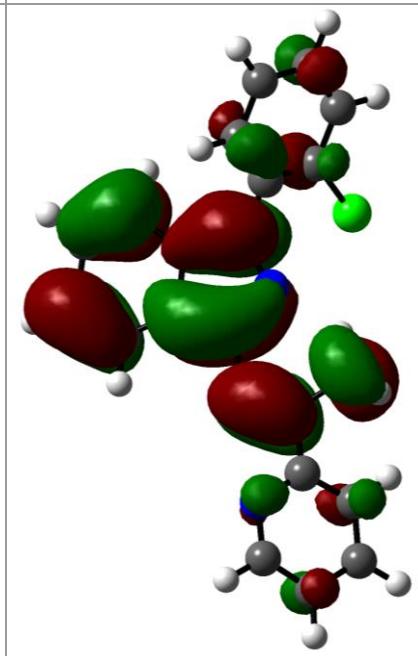
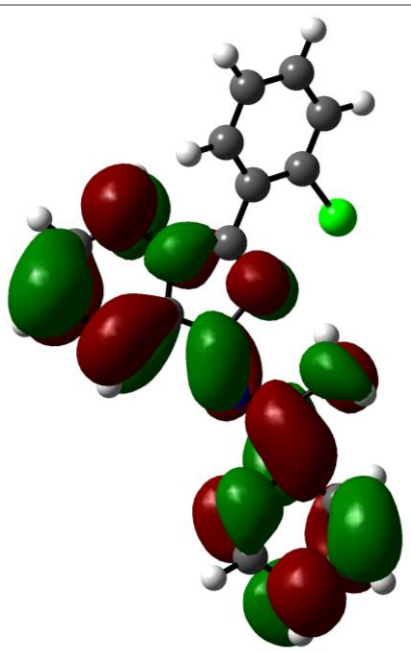
3o **3p**

Figure S35: DFT Optimized structure of b and **3p**.

Frontier molecular orbitals analysis:

Table S28: HOMO–LUMO diagrams and energy gap in **L1H**–**L5H**.

Entity	HOMO	LUMO	E_{HUMO} (eV)	E_{LOMO} (eV)	ΔE (eV)

L2H			-4.639	-1.318	3.321
L3H			-4.805	-1.355	3.450

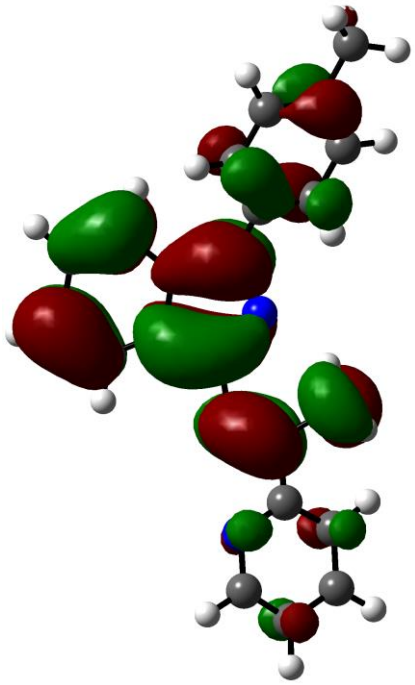
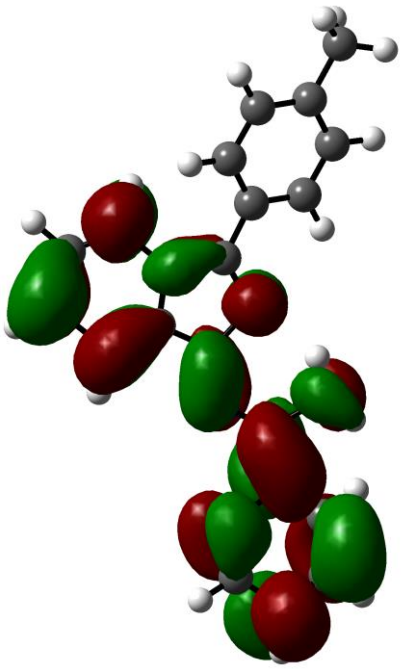
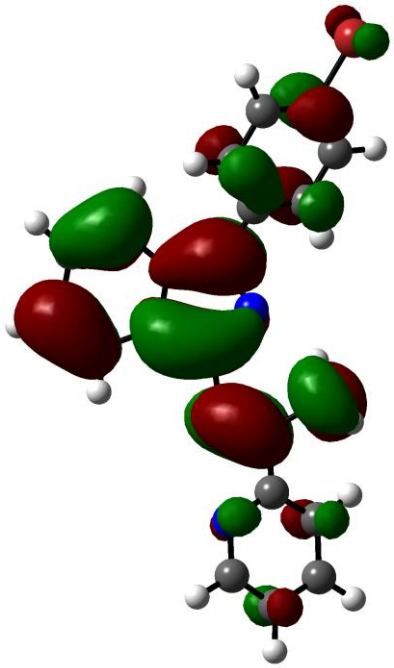
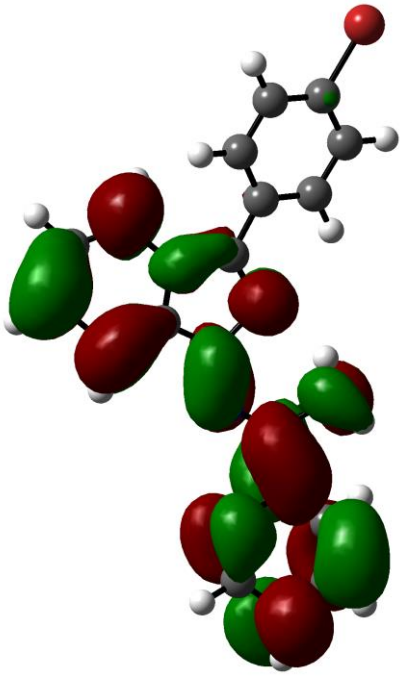
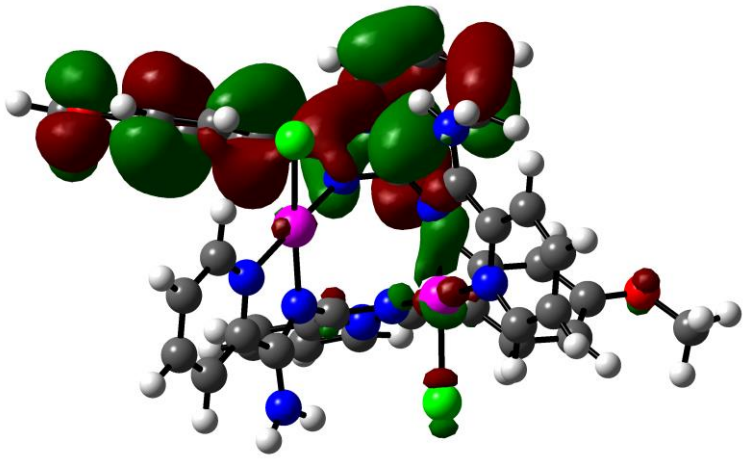
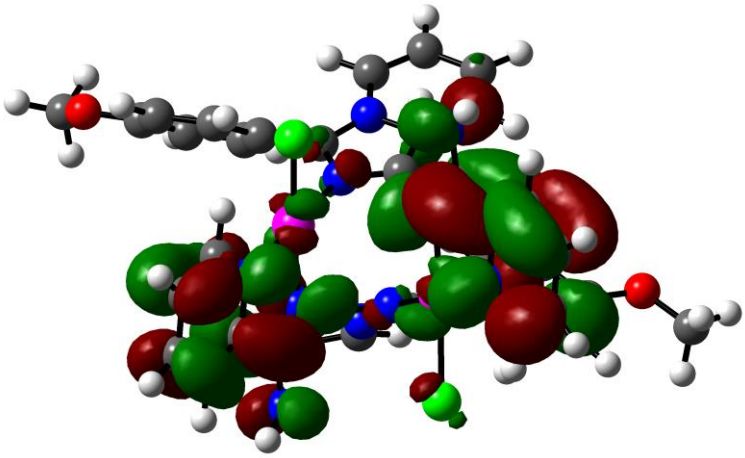
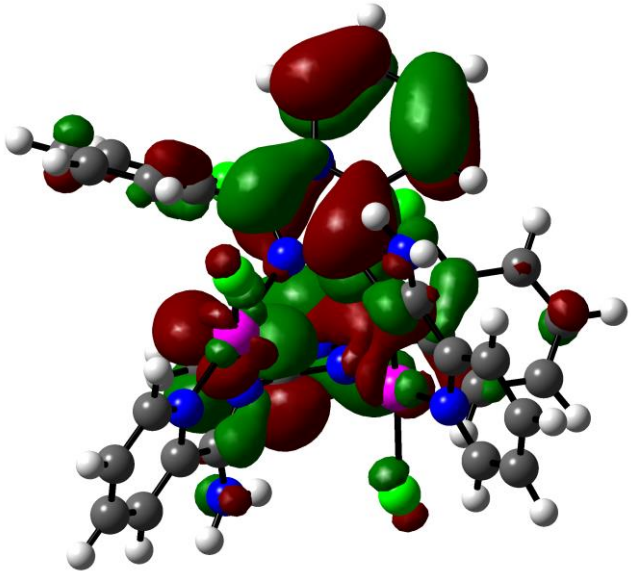
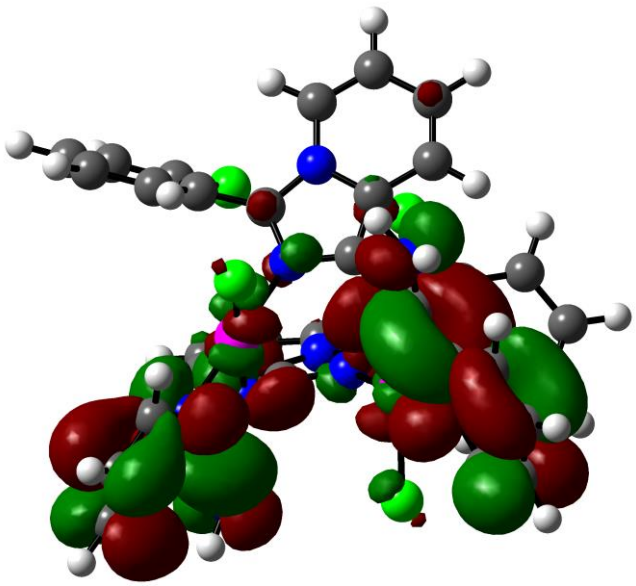
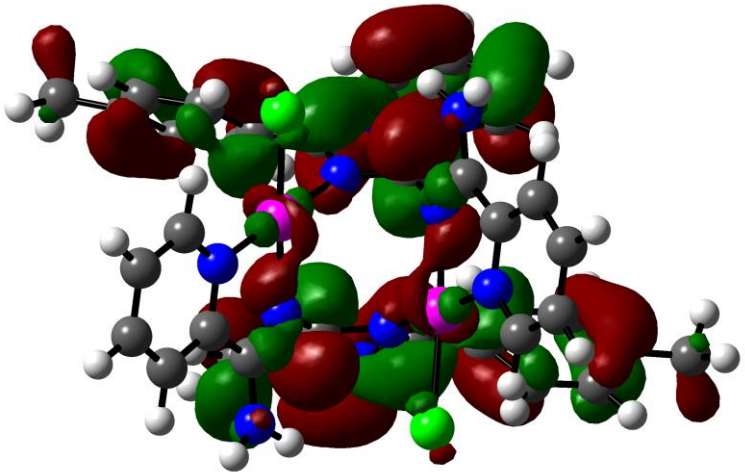
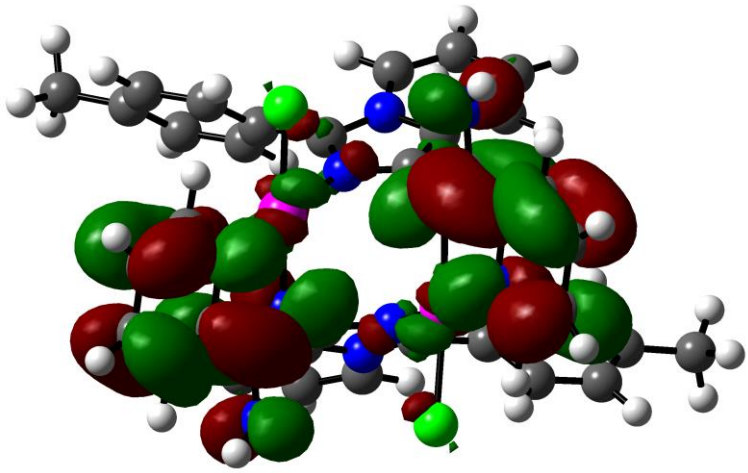
L4H			-4.704	-1.349	3.355
L5H			-4.885	-1.484	3.401

Table S29: HOMO–LUMO diagrams and energy calculations in **1** – **5**

Complexes		**HOMO/ LUMO**	**ΔE** (eV)

2		HOMO= −10.067	2.539
		LUMO= −7.528	
3		HOMO= −10.576	2.954

		**LUMO** = −7.622	
4		HOMO= −10.358	2.796
		LUMO= −7.562	

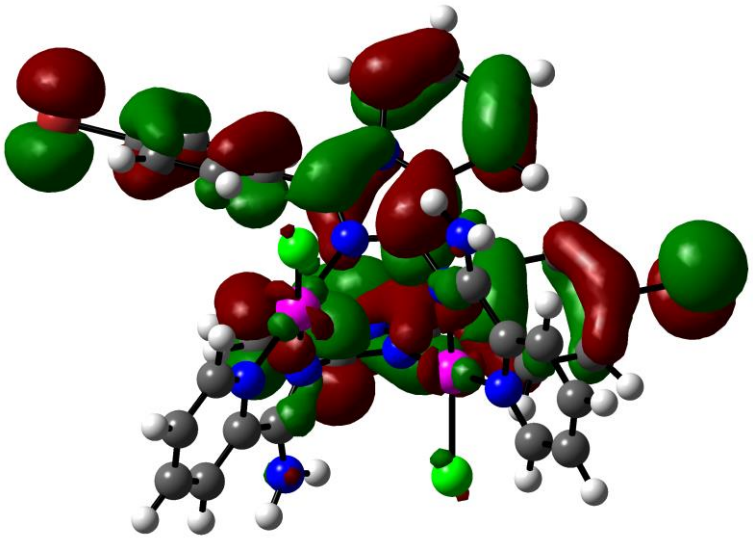
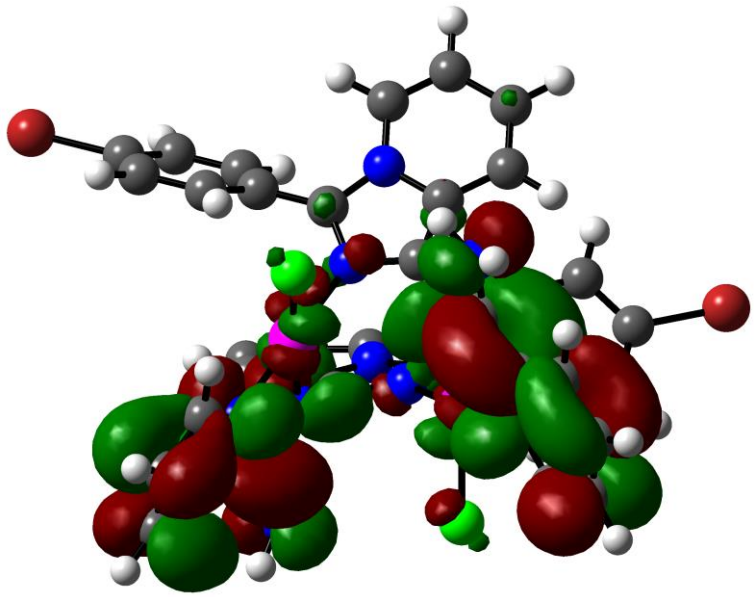
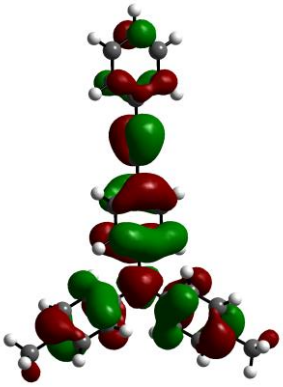
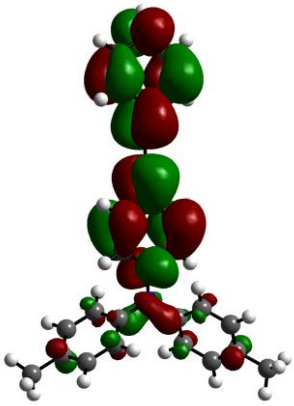
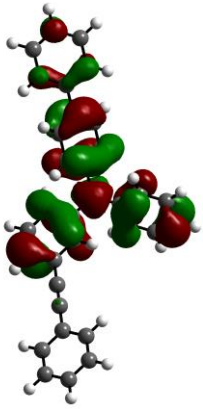
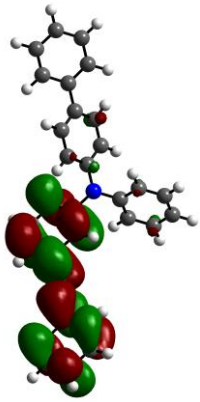
5		HOMO= −10.547	2.827
		LUMO= −7.720	

Table S30: HOMO–LUMO diagrams and energy gap in **3o** and **3p**.

Entity	HOMO	LUMO	E_{HUMO} (eV)	E_{LOMO} (eV)	ΔE (eV)

3o			-5.034	-1.344	3.69
3p			-5.231	-1.502	3.729

NBO analysis:

Table S31: Thermodynamic properties of **1–5**:

	1	**2**	**3**	**4**	**5**
Zero-point vibrational energy (Kcal/Mol)	436.4	436.1	383.4	430.4	382.6
Sum of electronic and zero-point Energies (Hartree)	-2524.8	-2524.8	-2324.5	-2374.4	-2320.9
Sum of electronic and thermal Energies (Hartree)	-2524.7	-2524.7	-2324.5	-2374.3	-2320.9
Sum of electronic and thermal Enthalpies (Hartree)	-2524.7	-2524.7	-2324.5	-2374.35	-2320.9
Sum of electronic and thermal Free Energies (Hartree)	-2524.9	-2524.9	-2324.6	-2374.5	-2321.0

Summary of natural population analysis of complex 1:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.14198	1.99893	3.83530	0.02379	5.85802

C	2	-0.22328	1.99907	4.20874	0.01547	6.22328
C	3	-0.18406	1.99918	4.17013	0.01475	6.18406
C	4	-0.23392	1.99918	4.22044	0.01429	6.23392
C	5	0.05925	1.99910	3.92394	0.01772	5.94075
C	6	0.48376	1.99893	3.48421	0.03309	5.51624
C	7	0.31717	1.99880	3.65390	0.03013	5.68283
H	8	0.24614	0.00000	0.75298	0.00089	0.75386
H	9	0.24510	0.00000	0.75416	0.00073	0.75490
H	10	0.25192	0.00000	0.74740	0.00067	0.74808
H	11	0.24703	0.00000	0.75158	0.00139	0.75297
C	12	0.54689	1.99892	3.43297	0.02122	5.45311
C	13	0.18382	1.99891	3.79344	0.02383	5.81618
C	14	-0.20425	1.99908	4.19058	0.01458	6.20425
C	15	-0.13363	1.99917	4.12097	0.01349	6.13363
H	16	0.23891	0.00000	0.76018	0.00090	0.76109
C	17	0.12503	1.99914	3.86022	0.01561	5.87497
C	18	-0.19923	1.99918	4.18592	0.01413	6.19923
H	19	0.25641	0.00000	0.74278	0.00081	0.74359
H	20	0.25944	0.00000	0.73982	0.00073	0.74056
C	21	-0.17402	1.99892	4.15098	0.02413	6.17402
C	22	-0.16604	1.99913	4.15157	0.01535	6.16604
C	23	0.34780	1.99874	3.63405	0.01941	5.65220
C	24	-0.22016	1.99915	4.20672	0.01430	6.22016
H	25	0.24546	0.00000	0.75327	0.00127	0.75454
C	26	-0.29057	1.99907	4.27757	0.01393	6.29057
C	27	-0.16114	1.99917	4.14824	0.01373	6.16114
H	28	0.23731	0.00000	0.76184	0.00085	0.76269
H	29	0.23466	0.00000	0.76433	0.00102	0.76534
N	30	-0.38587	1.99927	5.37730	0.00931	7.38587
N	31	-0.51379	1.99932	5.49429	0.02017	7.51379
N	32	-0.57205	1.99932	5.55094	0.02179	7.57205
N	33	-0.78378	1.99946	5.77259	0.01173	7.78378
H	34	0.43545	0.00000	0.56370	0.00085	0.56455
H	35	0.44937	0.00000	0.54883	0.00180	0.55063
N	36	-0.47753	1.99937	5.45969	0.01847	7.47753
Pd	37	0.53500	35.98828	9.46671	0.01001	45.46500
H	38	0.25868	0.00000	0.73962	0.00169	0.74132
C	39	0.14195	1.99893	3.83533	0.02379	5.85805
C	40	-0.22330	1.99907	4.20875	0.01547	6.22330
C	41	-0.18404	1.99918	4.17012	0.01475	6.18404
C	42	-0.23391	1.99918	4.22044	0.01429	6.23391
C	43	0.05924	1.99910	3.92394	0.01772	5.94076
C	44	0.48377	1.99893	3.48420	0.03309	5.51623

C	45	0.31717	1.99880	3.65391	0.03013	5.68283
H	46	0.24614	0.00000	0.75298	0.00089	0.75386
H	47	0.24510	0.00000	0.75416	0.00073	0.75490
H	48	0.25192	0.00000	0.74740	0.00067	0.74808
H	49	0.24703	0.00000	0.75158	0.00139	0.75297
C	50	0.54688	1.99892	3.43298	0.02122	5.45312
C	51	0.18382	1.99891	3.79344	0.02383	5.81618
C	52	-0.20424	1.99908	4.19057	0.01458	6.20424
C	53	-0.13363	1.99917	4.12097	0.01349	6.13363
H	54	0.23891	0.00000	0.76019	0.00090	0.76109
C	55	0.12503	1.99914	3.86022	0.01561	5.87497
C	56	-0.19922	1.99918	4.18591	0.01413	6.19922
H	57	0.25641	0.00000	0.74278	0.00081	0.74359
H	58	0.25944	0.00000	0.73982	0.00073	0.74056
C	59	-0.17403	1.99892	4.15098	0.02413	6.17403
C	60	-0.16604	1.99913	4.15156	0.01535	6.16604
C	61	0.34781	1.99874	3.63404	0.01941	5.65219
C	62	-0.22017	1.99915	4.20672	0.01430	6.22017
H	63	0.24547	0.00000	0.75327	0.00127	0.75453
C	64	-0.29058	1.99907	4.27759	0.01393	6.29058
C	65	-0.16114	1.99917	4.14824	0.01373	6.16114
H	66	0.23731	0.00000	0.76184	0.00085	0.76269
H	67	0.23465	0.00000	0.76433	0.00102	0.76535
N	68	-0.38587	1.99927	5.37729	0.00931	7.38587
N	69	-0.51379	1.99932	5.49429	0.02017	7.51379
N	70	-0.57205	1.99932	5.55094	0.02179	7.57205
N	71	-0.78379	1.99946	5.77259	0.01173	7.78379
H	72	0.43546	0.00000	0.56369	0.00085	0.56454
H	73	0.44937	0.00000	0.54883	0.00180	0.55063
N	74	-0.47752	1.99937	5.45969	0.01847	7.47752
Pd	75	0.53501	35.98828	9.46670	0.01001	45.46499
H	76	0.25868	0.00000	0.73963	0.00169	0.74132
Cl	77	-0.44328	10.00000	7.44267	0.00061	17.44328
Cl	78	-0.44332	10.00000	7.44271	0.00061	17.44332
H	79	0.23829	0.00000	0.76083	0.00088	0.76171
H	80	0.23829	0.00000	0.76083	0.00088	0.76171
C	81	-0.25982	1.99922	4.25244	0.00817	6.25982
H	82	0.22115	0.00000	0.77821	0.00064	0.77885
H	83	0.20052	0.00000	0.79796	0.00152	0.79948
H	84	0.20474	0.00000	0.79384	0.00142	0.79526
C	85	-0.25982	1.99922	4.25244	0.00817	6.25982
H	86	0.22115	0.00000	0.77821	0.00064	0.77885
H	87	0.20052	0.00000	0.79795	0.00152	0.79948

H	88	0.20473	0.00000	0.79385	0.00142	0.79527
O	89	-0.58481	1.99982	6.57561	0.00939	8.58481
O	90	-0.58483	1.99982	6.57562	0.00939	8.58483

Atom	No.	Natural electron configuration
C	1	[core]2S(0.86)2p(2.98)3p(0.02)
C	2	[core]2S(0.97)2p(3.23)3p(0.01)
C	3	[core]2S(0.99)2p(3.18)3p(0.01)
C	4	[core]2S(0.99)2p(3.23)3p(0.01)
C	5	[core]2S(0.94)2p(2.99)3p(0.02)
C	6	[core]2S(0.78)2p(2.70)3p(0.03)
C	7	[core]2S(0.77)2p(2.88)3p(0.03)
H	8	1S(0.75)
H	9	1S(0.75)
H	10	1S(0.75)
H	11	1S(0.75)
C	12	[core]2S(0.79)2p(2.64)3p(0.02)
C	13	[core]2S(0.86)2p(2.94)3p(0.02)
C	14	[core]2S(0.98)2p(3.21)3p(0.01)
C	15	[core]2S(1.00)2p(3.12)3p(0.01)
H	16	1S(0.76)
C	17	[core]2S(0.95)2p(2.91)3p(0.01)
C	18	[core]2S(1.00)2p(3.18)3p(0.01)
H	19	1S(0.74)
H	20	1S(0.74)
C	21	[core]2S(0.89)2p(3.26)3p(0.02)
C	22	[core]2S(0.97)2p(3.18)3p(0.01)
C	23	[core]2S(0.84)2p(2.79)3p(0.02)
C	24	[core]2S(0.98)2p(3.23)3p(0.01)
H	25	1S(0.75)
C	26	[core]2S(0.98)2p(3.30)3p(0.01)
C	27	[core]2S(0.98)2p(3.16)3p(0.01)
H	28	1S(0.76)
H	29	1S(0.76)
N	30	[core]2S(1.22)2p(4.16)3p(0.01)
N	31	[core]2S(1.34)2p(4.16)3p(0.02)
N	32	[core]2S(1.30)2p(4.25)3p(0.02)
N	33	[core]2S(1.32)2p(4.45)3p(0.01)
H	34	1S(0.56)
H	35	1S(0.55)
N	36	[core]2S(1.33)2p(4.13)3p(0.02)
Pd	37	[core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)
H	38	1S(0.74)

C 39 [core]2S(0.86)2p(2.98)3p(0.02)
C 40 [core]2S(0.97)2p(3.23)3p(0.01)
C 41 [core]2S(0.99)2p(3.18)3p(0.01)
C 42 [core]2S(0.99)2p(3.23)3p(0.01)
C 43 [core]2S(0.94)2p(2.99)3p(0.02)
C 44 [core]2S(0.78)2p(2.70)3p(0.03)
C 45 [core]2S(0.77)2p(2.88)3p(0.03)
H 46 1S(0.75)
H 47 1S(0.75)
H 48 1S(0.75)
H 49 1S(0.75)
C 50 [core]2S(0.79)2p(2.64)3p(0.02)
C 51 [core]2S(0.86)2p(2.94)3p(0.02)
C 52 [core]2S(0.98)2p(3.21)3p(0.01)
C 53 [core]2S(1.00)2p(3.12)3p(0.01)
H 54 1S(0.76)
C 55 [core]2S(0.95)2p(2.91)3p(0.01)
C 56 [core]2S(1.00)2p(3.18)3p(0.01)
H 57 1S(0.74)
H 58 1S(0.74)
C 59 [core]2S(0.89)2p(3.26)3p(0.02)
C 60 [core]2S(0.97)2p(3.18)3p(0.01)
C 61 [core]2S(0.84)2p(2.79)3p(0.02)
C 62 [core]2S(0.98)2p(3.23)3p(0.01)
H 63 1S(0.75)
C 64 [core]2S(0.98)2p(3.30)3p(0.01)
C 65 [core]2S(0.98)2p(3.16)3p(0.01)
H 66 1S(0.76)
H 67 1S(0.76)
N 68 [core]2S(1.22)2p(4.16)3p(0.01)
N 69 [core]2S(1.34)2p(4.16)3p(0.02)
N 70 [core]2S(1.30)2p(4.25)3p(0.02)
N 71 [core]2S(1.32)2p(4.45)3p(0.01)
H 72 1S(0.56)
H 73 1S(0.55)
N 74 [core]2S(1.33)2p(4.13)3p(0.02)
Pd 75 [core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)
H 76 1S(0.74)
Cl 77 [core]3S(1.90)3p(5.54)
Cl 78 [core]3S(1.90)3p(5.54)
H 79 1S(0.76)
H 80 1S(0.76)
C 81 [core]2S(1.10)2p(3.15)3p(0.01)

	H	82	1S(0.78)
	H	83	1S(0.80)
	H	84	1S(0.79)
C	85	[core]2S(1.10)2p(3.15)3p(0.01)	
	H	86	1S(0.78)
	H	87	1S(0.80)
	H	88	1S(0.79)
O	89	[core]2S(1.64)2p(4.94)3p(0.01)	
O	90	[core]2S(1.64)2p(4.94)3p(0.01)	

Summary of natural population analysis of complex 2:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.14086	1.99893	3.83718	0.02304	5.85914
C	2	-0.21935	1.99908	4.20498	0.01529	6.21935
C	3	-0.17902	1.99918	4.16547	0.01438	6.17902
C	4	-0.22613	1.99919	4.21280	0.01415	6.22613
C	5	0.04036	1.99910	3.94450	0.01605	5.95964
C	6	0.47839	1.99892	3.49199	0.03070	5.52161
C	7	0.31376	1.99880	3.65736	0.03007	5.68624
H	8	0.24746	0.00000	0.75166	0.00088	0.75254
H	9	0.24643	0.00000	0.75283	0.00074	0.75357
H	10	0.25457	0.00000	0.74475	0.00068	0.74543
H	11	0.24887	0.00000	0.75000	0.00113	0.75113
C	12	0.54818	1.99892	3.43182	0.02108	5.45182
C	13	0.18305	1.99891	3.79424	0.02380	5.81695
C	14	-0.20381	1.99908	4.19017	0.01455	6.20381
C	15	-0.13333	1.99917	4.12066	0.01350	6.13333
H	16	0.23912	0.00000	0.75998	0.00090	0.76088
C	17	0.12524	1.99914	3.86002	0.01560	5.87476
C	18	-0.19822	1.99918	4.18491	0.01413	6.19822
H	19	0.25681	0.00000	0.74238	0.00081	0.74319
H	20	0.26003	0.00000	0.73924	0.00073	0.73997
C	21	-0.16143	1.99897	4.14091	0.02155	6.16143
C	22	-0.16180	1.99912	4.14695	0.01572	6.16180
C	23	-0.20182	1.99910	4.18809	0.01462	6.20182
C	24	-0.28888	1.99908	4.27603	0.01377	6.28888
H	25	0.24480	0.00000	0.75391	0.00130	0.75520
C	26	-0.23074	1.99907	4.21448	0.01719	6.23074
C	27	0.36400	1.99885	3.61780	0.01936	5.63600
H	28	0.23649	0.00000	0.76255	0.00096	0.76351
H	29	0.24774	0.00000	0.75111	0.00114	0.75226

N	30	-0.40021	1.99928	5.39186	0.00907	7.40021
N	31	-0.51847	1.99933	5.49894	0.02021	7.51847
N	32	-0.57411	1.99932	5.55309	0.02170	7.57411
N	33	-0.78167	1.99946	5.77053	0.01169	7.78167
H	34	0.43559	0.00000	0.56357	0.00085	0.56441
H	35	0.45114	0.00000	0.54696	0.00190	0.54886
N	36	-0.47770	1.99937	5.45991	0.01842	7.47770
Pd	37	0.53076	35.98843	9.47080	0.01001	45.46924
H	38	0.25907	0.00000	0.73925	0.00168	0.74093
C	39	0.14099	1.99893	3.83703	0.02306	5.85901
C	40	-0.21917	1.99908	4.20475	0.01534	6.21917
C	41	-0.17730	1.99918	4.16371	0.01441	6.17730
C	42	-0.22529	1.99918	4.21197	0.01414	6.22529
C	43	0.03918	1.99910	3.94568	0.01604	5.96082
C	44	0.47763	1.99892	3.49312	0.03033	5.52237
C	45	0.31401	1.99880	3.65714	0.03005	5.68599
H	46	0.24745	0.00000	0.75167	0.00088	0.75255
H	47	0.24788	0.00000	0.75139	0.00074	0.75212
H	48	0.25474	0.00000	0.74458	0.00068	0.74526
H	49	0.24741	0.00000	0.75147	0.00113	0.75259
C	50	0.54809	1.99892	3.43189	0.02111	5.45191
C	51	0.18360	1.99891	3.79367	0.02381	5.81640
C	52	-0.20375	1.99908	4.19011	0.01456	6.20375
C	53	-0.13353	1.99917	4.12087	0.01350	6.13353
H	54	0.23929	0.00000	0.75981	0.00090	0.76071
C	55	0.12435	1.99914	3.86092	0.01558	5.87565
C	56	-0.19928	1.99918	4.18597	0.01413	6.19928
H	57	0.25676	0.00000	0.74242	0.00081	0.74324
H	58	0.25960	0.00000	0.73966	0.00073	0.74040
C	59	-0.15779	1.99897	4.13736	0.02146	6.15779
C	60	-0.17511	1.99913	4.16047	0.01551	6.17511
C	61	-0.19017	1.99910	4.17591	0.01515	6.19017
C	62	-0.22643	1.99907	4.21070	0.01667	6.22643
H	63	0.24376	0.00000	0.75500	0.00124	0.75624
C	64	-0.29162	1.99908	4.27830	0.01424	6.29162
C	65	0.36443	1.99885	3.61739	0.01933	5.63557
H	66	0.24926	0.00000	0.74962	0.00112	0.75074
H	67	0.23487	0.00000	0.76417	0.00096	0.76513
N	68	-0.40056	1.99929	5.39221	0.00906	7.40056
N	69	-0.51974	1.99933	5.50022	0.02019	7.51974
N	70	-0.57413	1.99932	5.55313	0.02168	7.57413
N	71	-0.78065	1.99946	5.76949	0.01170	7.78065
H	72	0.43544	0.00000	0.56371	0.00085	0.56456

H	73	0.45169	0.00000	0.54638	0.00193	0.54831
N	74	-0.47817	1.99937	5.46042	0.01838	7.47817
Pd	75	0.53203	35.98844	9.46950	0.01003	45.46797
H	76	0.25867	0.00000	0.73964	0.00169	0.74133
Cl	77	-0.44134	10.00000	7.44072	0.00062	17.44134
Cl	78	-0.44347	10.00000	7.44286	0.00062	17.44347
H	79	0.22301	0.00000	0.77591	0.00108	0.77699
H	80	0.22384	0.00000	0.77517	0.00099	0.77616
C	81	-0.26335	1.99922	4.25699	0.00715	6.26335
H	82	0.19606	0.00000	0.80246	0.00149	0.80394
H	83	0.20234	0.00000	0.79621	0.00145	0.79766
H	84	0.23482	0.00000	0.76466	0.00052	0.76518
C	85	-0.26357	1.99922	4.25720	0.00715	6.26357
H	86	0.19511	0.00000	0.80339	0.00150	0.80489
H	87	0.23566	0.00000	0.76382	0.00053	0.76434
H	88	0.20107	0.00000	0.79747	0.00146	0.79893
O	89	-0.54808	1.99982	6.53766	0.01060	8.54808
O	90	-0.54654	1.99982	6.53609	0.01063	8.54654

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.86)2p(2.98)3p(0.02)
C	2	[core]2S(0.98)2p(3.23)3p(0.01)
C	3	[core]2S(0.99)2p(3.18)3p(0.01)
C	4	[core]2S(0.99)2p(3.22)3p(0.01)
C	5	[core]2S(0.94)2p(3.01)3p(0.01)
C	6	[core]2S(0.79)2p(2.70)3p(0.03)
C	7	[core]2S(0.78)2p(2.88)3p(0.03)
H	8	1S(0.75)
H	9	1S(0.75)
H	10	1S(0.74)
H	11	1S(0.75)
C	12	[core]2S(0.79)2p(2.64)3p(0.02)
C	13	[core]2S(0.86)2p(2.94)3p(0.02)
C	14	[core]2S(0.98)2p(3.21)3p(0.01)
C	15	[core]2S(1.00)2p(3.12)3p(0.01)
H	16	1S(0.76)
C	17	[core]2S(0.95)2p(2.91)3p(0.01)
C	18	[core]2S(1.00)2p(3.18)3p(0.01)
H	19	1S(0.74)
H	20	1S(0.74)
C	21	[core]2S(0.89)2p(3.25)3p(0.02)
C	22	[core]2S(0.97)2p(3.18)3p(0.01)

C 23 [core]2S(0.97)2p(3.22)3p(0.01)
C 24 [core]2S(0.98)2p(3.30)3p(0.01)
H 25 1S(0.75)
C 26 [core]2S(0.98)2p(3.23)3p(0.02)
C 27 [core]2S(0.85)2p(2.76)3p(0.02)
H 28 1S(0.76)
H 29 1S(0.75)
N 30 [core]2S(1.22)2p(4.17)3p(0.01)
N 31 [core]2S(1.34)2p(4.16)3p(0.02)
N 32 [core]2S(1.30)2p(4.25)3p(0.02)
N 33 [core]2S(1.32)2p(4.45)3p(0.01)
H 34 1S(0.56)
H 35 1S(0.55)
N 36 [core]2S(1.33)2p(4.13)3p(0.02)
Pd 37 [core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)
H 38 1S(0.74)
C 39 [core]2S(0.86)2p(2.98)3p(0.02)
C 40 [core]2S(0.98)2p(3.23)3p(0.01)
C 41 [core]2S(0.99)2p(3.17)3p(0.01)
C 42 [core]2S(0.99)2p(3.22)3p(0.01)
C 43 [core]2S(0.94)2p(3.01)3p(0.01)
C 44 [core]2S(0.79)2p(2.71)3p(0.03)
C 45 [core]2S(0.78)2p(2.88)3p(0.03)
H 46 1S(0.75)
H 47 1S(0.75)
H 48 1S(0.74)
H 49 1S(0.75)
C 50 [core]2S(0.79)2p(2.64)3p(0.02)
C 51 [core]2S(0.86)2p(2.94)3p(0.02)
C 52 [core]2S(0.98)2p(3.21)3p(0.01)
C 53 [core]2S(1.00)2p(3.12)3p(0.01)
H 54 1S(0.76)
C 55 [core]2S(0.95)2p(2.91)3p(0.01)
C 56 [core]2S(1.00)2p(3.18)3p(0.01)
H 57 1S(0.74)
H 58 1S(0.74)
C 59 [core]2S(0.89)2p(3.25)3p(0.02)
C 60 [core]2S(0.97)2p(3.19)3p(0.01)
C 61 [core]2S(0.97)2p(3.21)3p(0.01)
C 62 [core]2S(0.98)2p(3.23)3p(0.01)
H 63 1S(0.75)
C 64 [core]2S(0.98)2p(3.30)3p(0.01)
C 65 [core]2S(0.85)2p(2.76)3p(0.02)

	H	66	1S(0.75)
	H	67	1S(0.76)
N	68	[core]2S(1.22)2p(4.17)3p(0.01)	
N	69	[core]2S(1.34)2p(4.16)3p(0.02)	
N	70	[core]2S(1.30)2p(4.25)3p(0.02)	
N	71	[core]2S(1.32)2p(4.44)3p(0.01)	
	H	72	1S(0.56)
	H	73	1S(0.55)
N	74	[core]2S(1.33)2p(4.13)3p(0.02)	
Pd	75	[core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)	
	H	76	1S(0.74)
Cl	77	[core]3S(1.90)3p(5.54)	
Cl	78	[core]3S(1.90)3p(5.54)	
	H	79	1S(0.78)
	H	80	1S(0.78)
C	81	[core]2S(1.11)2p(3.15)3p(0.01)	
	H	82	1S(0.80)
	H	83	1S(0.80)
	H	84	1S(0.76)
C	85	[core]2S(1.11)2p(3.15)3p(0.01)	
	H	86	1S(0.80)
	H	87	1S(0.76)
	H	88	1S(0.80)
O	89	[core]2S(1.64)2p(4.90)3p(0.01)	
O	90	[core]2S(1.64)2p(4.90)3p(0.01)	

Summary of natural population analysis of complex 3:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.07159	0.99947	1.91709	0.01185	2.92841
C	2	-0.11168	0.99954	2.10428	0.00787	3.11168
C	3	-0.08410	0.99959	2.07733	0.00718	3.08410
C	4	-0.10883	0.99959	2.10216	0.00707	3.10883
C	5	0.02371	0.99955	1.96813	0.00861	2.97629
C	6	0.23405	0.99946	1.74964	0.01685	2.76595
C	7	0.15880	0.99940	1.82668	0.01512	2.84120
H	8	0.12307	0.00000	0.37649	0.00044	0.37693
H	9	0.12397	0.00000	0.37566	0.00037	0.37603
H	10	0.12816	0.00000	0.37150	0.00033	0.37184
H	11	0.12377	0.00000	0.37556	0.00067	0.37623
C	12	0.27283	0.99946	1.71710	0.01061	2.72717
C	13	0.09155	0.99946	1.89710	0.01190	2.90845

C	14	-0.10190	0.99954	2.09506	0.00729	3.10190
C	15	-0.06622	0.99958	2.05988	0.00675	3.06622
H	16	0.11960	0.00000	0.37995	0.00045	0.38040
C	17	0.06265	0.99957	1.92998	0.00781	2.93735
C	18	-0.09921	0.99959	2.09256	0.00707	3.09921
H	19	0.12862	0.00000	0.37098	0.00041	0.37138
H	20	0.13010	0.00000	0.36954	0.00037	0.36990
C	21	-0.07938	0.99941	2.06853	0.01144	3.07938
C	22	-0.08211	0.99955	2.07516	0.00740	3.08211
C	23	0.01000	0.99932	1.98002	0.01066	2.99000
C	24	-0.09891	0.99958	2.09245	0.00688	3.09891
H	25	0.12539	0.00000	0.37395	0.00066	0.37461
C	26	-0.11028	0.99948	2.10268	0.00811	3.11028
C	27	-0.08326	0.99958	2.07718	0.00649	3.08326
H	28	0.12103	0.00000	0.37851	0.00045	0.37897
H	29	0.12711	0.00000	0.37235	0.00054	0.37289
H	30	0.12204	0.00000	0.37753	0.00042	0.37796
Cl	31	-0.02518	5.00000	3.52406	0.00112	8.52518
N	32	-0.19377	0.99963	2.68952	0.00462	3.69377
N	33	-0.25523	0.99966	2.74548	0.01009	3.75523
N	34	-0.28711	0.99966	2.77654	0.01091	3.78711
N	35	-0.39180	0.99973	2.88619	0.00588	3.89180
H	36	0.21800	0.00000	0.28158	0.00042	0.28200
H	37	0.22478	0.00000	0.27430	0.00092	0.27522
N	38	-0.23896	0.99968	2.73010	0.00918	3.73896
Pd	39	0.26912	17.99422	4.73172	0.00493	22.73088
H	40	0.12943	0.00000	0.36974	0.00083	0.37057
C	41	0.07157	0.99947	1.91712	0.01185	2.92843
C	42	-0.11169	0.99954	2.10428	0.00787	3.11169
C	43	-0.08410	0.99959	2.07733	0.00718	3.08410
C	44	-0.10882	0.99959	2.10216	0.00707	3.10882
C	45	0.02371	0.99955	1.96813	0.00861	2.97629
C	46	0.23406	0.99946	1.74963	0.01685	2.76594
C	47	0.15881	0.99940	1.82667	0.01512	2.84119
H	48	0.12307	0.00000	0.37649	0.00044	0.37693
H	49	0.12397	0.00000	0.37566	0.00037	0.37603
H	50	0.12816	0.00000	0.37150	0.00033	0.37184
H	51	0.12377	0.00000	0.37556	0.00067	0.37623
C	52	0.27282	0.99946	1.71711	0.01061	2.72718
C	53	0.09155	0.99946	1.89710	0.01190	2.90845
C	54	-0.10190	0.99954	2.09506	0.00729	3.10190
C	55	-0.06622	0.99958	2.05989	0.00675	3.06622
H	56	0.11960	0.00000	0.37995	0.00045	0.38040

C	57	0.06264	0.99957	1.92998	0.00781	2.93736
C	58	-0.09921	0.99959	2.09255	0.00707	3.09921
H	59	0.12862	0.00000	0.37098	0.00041	0.37138
H	60	0.13010	0.00000	0.36954	0.00037	0.36990
C	61	-0.07939	0.99941	2.06853	0.01144	3.07939
C	62	-0.08211	0.99955	2.07515	0.00740	3.08211
C	63	0.01000	0.99932	1.98002	0.01066	2.99000
C	64	-0.09891	0.99958	2.09246	0.00688	3.09891
H	65	0.12539	0.00000	0.37395	0.00066	0.37461
C	66	-0.11028	0.99948	2.10268	0.00811	3.11028
C	67	-0.08326	0.99958	2.07718	0.00649	3.08326
H	68	0.12103	0.00000	0.37851	0.00045	0.37897
H	69	0.12711	0.00000	0.37235	0.00054	0.37289
H	70	0.12204	0.00000	0.37753	0.00042	0.37796
Cl	71	-0.02518	5.00000	3.52406	0.00112	8.52518
N	72	-0.19376	0.99963	2.68951	0.00462	3.69376
N	73	-0.25524	0.99966	2.74549	0.01009	3.75524
N	74	-0.28710	0.99966	2.77653	0.01091	3.78710
N	75	-0.39182	0.99973	2.88620	0.00588	3.89182
H	76	0.21799	0.00000	0.28159	0.00042	0.28201
H	77	0.22478	0.00000	0.27430	0.00092	0.27522
N	78	-0.23896	0.99968	2.73010	0.00918	3.73896
Pd	79	0.26910	17.99422	4.73175	0.00493	22.73090
H	80	0.12943	0.00000	0.36974	0.00083	0.37057
Cl	81	-0.22143	5.00000	3.72112	0.00031	8.72143
Cl	82	-0.22141	5.00000	3.72110	0.00031	8.72141

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.43)2p(1.49)3p(0.01)
C	2	[core]2S(0.49)2p(1.62)3p(0.01)
C	3	[core]2S(0.49)2p(1.58)3p(0.01)
C	4	[core]2S(0.50)2p(1.61)3p(0.01)
C	5	[core]2S(0.47)2p(1.50)3p(0.01)
C	6	[core]2S(0.39)2p(1.36)3p(0.02)
C	7	[core]2S(0.39)2p(1.44)3p(0.01)
H	8	1S(0.38)
H	9	1S(0.38)
H	10	1S(0.37)
H	11	1S(0.38)
C	12	[core]2S(0.40)2p(1.32)3p(0.01)
C	13	[core]2S(0.43)2p(1.47)3p(0.01)
C	14	[core]2S(0.49)2p(1.60)3p(0.01)

C 15 [core]2S(0.50)2p(1.56)3p(0.01)
H 16 1S(0.38)
C 17 [core]2S(0.48)2p(1.45)3p(0.01)
C 18 [core]2S(0.50)2p(1.59)3p(0.01)
H 19 1S(0.37)
H 20 1S(0.37)
C 21 [core]2S(0.45)2p(1.62)3p(0.01)
C 22 [core]2S(0.49)2p(1.59)3p(0.01)
C 23 [core]2S(0.48)2p(1.50)3p(0.01)
C 24 [core]2S(0.49)2p(1.60)3p(0.01)
H 25 1S(0.37)
C 26 [core]2S(0.49)2p(1.61)3p(0.01)
C 27 [core]2S(0.50)2p(1.58)3p(0.01)
H 28 1S(0.38)
H 29 1S(0.37)
H 30 1S(0.38)
Cl 31 [core]3S(0.93)3p(2.60)
N 32 [core]2S(0.61)2p(2.08)
N 33 [core]2S(0.67)2p(2.08)3p(0.01)
N 34 [core]2S(0.65)2p(2.12)3p(0.01)
N 35 [core]2S(0.66)2p(2.22)3p(0.01)
H 36 1S(0.28)
H 37 1S(0.27)
N 38 [core]2S(0.66)2p(2.07)3p(0.01)
Pd 39 [core]5S(0.16)4d(4.43)5p(0.14)
H 40 1S(0.37)
C 41 [core]2S(0.43)2p(1.49)3p(0.01)
C 42 [core]2S(0.49)2p(1.62)3p(0.01)
C 43 [core]2S(0.49)2p(1.58)3p(0.01)
C 44 [core]2S(0.50)2p(1.61)3p(0.01)
C 45 [core]2S(0.47)2p(1.50)3p(0.01)
C 46 [core]2S(0.39)2p(1.36)3p(0.02)
C 47 [core]2S(0.39)2p(1.44)3p(0.01)
H 48 1S(0.38)
H 49 1S(0.38)
H 50 1S(0.37)
H 51 1S(0.38)
C 52 [core]2S(0.40)2p(1.32)3p(0.01)
C 53 [core]2S(0.43)2p(1.47)3p(0.01)
C 54 [core]2S(0.49)2p(1.60)3p(0.01)
C 55 [core]2S(0.50)2p(1.56)3p(0.01)
H 56 1S(0.38)
C 57 [core]2S(0.48)2p(1.45)3p(0.01)

C	58	[core]2S(0.50)2p(1.59)3p(0.01)
H	59	1S(0.37)
H	60	1S(0.37)
C	61	[core]2S(0.45)2p(1.62)3p(0.01)
C	62	[core]2S(0.49)2p(1.59)3p(0.01)
C	63	[core]2S(0.48)2p(1.50)3p(0.01)
C	64	[core]2S(0.49)2p(1.60)3p(0.01)
H	65	1S(0.37)
C	66	[core]2S(0.49)2p(1.61)3p(0.01)
C	67	[core]2S(0.50)2p(1.58)3p(0.01)
H	68	1S(0.38)
H	69	1S(0.37)
H	70	1S(0.38)
Cl	71	[core]3S(0.93)3p(2.60)
N	72	[core]2S(0.61)2p(2.08)
N	73	[core]2S(0.67)2p(2.08)3p(0.01)
N	74	[core]2S(0.65)2p(2.12)3p(0.01)
N	75	[core]2S(0.66)2p(2.22)3p(0.01)
H	76	1S(0.28)
H	77	1S(0.27)
N	78	[core]2S(0.66)2p(2.07)3p(0.01)
Pd	79	[core]5S(0.16)4d(4.43)5p(0.14)
H	80	1S(0.37)
Cl	81	[core]3S(0.95)3p(2.77)
Cl	82	[core]3S(0.95)3p(2.77)

Summary of natural population analysis of complex 4:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.14156	1.99893	3.83647	0.02304	5.85844
C	2	-0.21903	1.99908	4.20466	0.01530	6.21903
C	3	-0.17735	1.99918	4.16381	0.01436	6.17735
C	4	-0.22478	1.99919	4.21148	0.01411	6.22478
C	5	0.04016	1.99910	3.94473	0.01601	5.95984
C	6	0.47774	1.99892	3.49269	0.03065	5.52226
C	7	0.31454	1.99880	3.65660	0.03005	5.68546
H	8	0.24764	0.00000	0.75148	0.00088	0.75236
H	9	0.24749	0.00000	0.75177	0.00074	0.75251
H	10	0.25513	0.00000	0.74420	0.00068	0.74487
H	11	0.24877	0.00000	0.75010	0.00113	0.75123
C	12	0.54827	1.99892	3.43171	0.02109	5.45173
C	13	0.18313	1.99891	3.79415	0.02380	5.81687
C	14	-0.20364	1.99908	4.19000	0.01455	6.20364

C	15	-0.13318	1.99917	4.12051	0.01350	6.13318
H	16	0.23933	0.00000	0.75977	0.00090	0.76067
C	17	0.12497	1.99914	3.86029	0.01559	5.87503
C	18	-0.19845	1.99918	4.18514	0.01413	6.19845
H	19	0.25699	0.00000	0.74220	0.00081	0.74301
H	20	0.26004	0.00000	0.73922	0.00073	0.73996
C	21	-0.14260	1.99897	4.12270	0.02093	6.14260
C	22	-0.17522	1.99911	4.16065	0.01546	6.17522
C	23	-0.20283	1.99909	4.18882	0.01492	6.20283
C	24	-0.20319	1.99904	4.19010	0.01405	6.20319
H	25	0.24288	0.00000	0.75584	0.00128	0.75712
C	26	-0.20862	1.99904	4.19520	0.01438	6.20862
C	27	0.03045	1.99908	3.95389	0.01658	5.96955
H	28	0.23256	0.00000	0.76632	0.00112	0.76744
H	29	0.23082	0.00000	0.76807	0.00111	0.76918
N	30	-0.39926	1.99929	5.39097	0.00900	7.39926
N	31	-0.51772	1.99933	5.49825	0.02014	7.51772
N	32	-0.57488	1.99932	5.55388	0.02168	7.57488
N	33	-0.78088	1.99946	5.76973	0.01169	7.78088
H	34	0.43570	0.00000	0.56345	0.00085	0.56430
H	35	0.45150	0.00000	0.54657	0.00193	0.54850
N	36	-0.47783	1.99937	5.46007	0.01839	7.47783
Pd	37	0.53221	35.98845	9.46939	0.00996	45.46779
H	38	0.25903	0.00000	0.73930	0.00168	0.74097
C	39	0.14156	1.99893	3.83647	0.02304	5.85844
C	40	-0.21904	1.99908	4.20466	0.01530	6.21904
C	41	-0.17735	1.99918	4.16381	0.01436	6.17735
C	42	-0.22478	1.99919	4.21148	0.01411	6.22478
C	43	0.04016	1.99910	3.94473	0.01601	5.95984
C	44	0.47774	1.99892	3.49269	0.03065	5.52226
C	45	0.31455	1.99880	3.65660	0.03005	5.68545
H	46	0.24764	0.00000	0.75148	0.00088	0.75236
H	47	0.24749	0.00000	0.75177	0.00074	0.75251
H	48	0.25513	0.00000	0.74420	0.00068	0.74487
H	49	0.24877	0.00000	0.75010	0.00113	0.75123
C	50	0.54827	1.99892	3.43172	0.02109	5.45173
C	51	0.18313	1.99891	3.79416	0.02380	5.81687
C	52	-0.20364	1.99908	4.19000	0.01455	6.20364
C	53	-0.13318	1.99917	4.12051	0.01350	6.13318
H	54	0.23933	0.00000	0.75977	0.00090	0.76067
C	55	0.12497	1.99914	3.86029	0.01559	5.87503
C	56	-0.19845	1.99918	4.18514	0.01413	6.19845
H	57	0.25699	0.00000	0.74219	0.00081	0.74301
H	58	0.26004	0.00000	0.73922	0.00073	0.73996
C	59	-0.14259	1.99897	4.12269	0.02093	6.14259
C	60	-0.17523	1.99911	4.16066	0.01546	6.17523
C	61	-0.20282	1.99909	4.18882	0.01492	6.20282

C	62	-0.20319	1.99904	4.19010	0.01404	6.20319
H	63	0.24288	0.00000	0.75584	0.00128	0.75712
C	64	-0.20863	1.99904	4.19520	0.01438	6.20863
C	65	0.03045	1.99908	3.95389	0.01658	5.96955
H	66	0.23256	0.00000	0.76632	0.00112	0.76744
H	67	0.23083	0.00000	0.76807	0.00111	0.76917
N	68	-0.39926	1.99929	5.39097	0.00900	7.39926
N	69	-0.51771	1.99933	5.49824	0.02014	7.51771
N	70	-0.57488	1.99932	5.55388	0.02168	7.57488
N	71	-0.78089	1.99946	5.76974	0.01169	7.78089
H	72	0.43570	0.00000	0.56345	0.00085	0.56430
H	73	0.45150	0.00000	0.54657	0.00193	0.54850
N	74	-0.47783	1.99937	5.46007	0.01839	7.47783
Pd	75	0.53222	35.98845	9.46938	0.00996	45.46778
H	76	0.25903	0.00000	0.73930	0.00168	0.74097
Cl	77	-0.44158	10.00000	7.44096	0.00062	17.44158
Cl	78	-0.44159	10.00000	7.44097	0.00062	17.44159
H	79	0.22169	0.00000	0.77723	0.00108	0.77831
H	80	0.22169	0.00000	0.77723	0.00108	0.77831
C	81	-0.65636	1.99927	4.64833	0.00876	6.65636
H	82	0.24829	0.00000	0.75058	0.00113	0.75171
H	83	0.23137	0.00000	0.76773	0.00090	0.76863
H	84	0.23513	0.00000	0.76395	0.00092	0.76487
C	85	-0.65636	1.99927	4.64833	0.00876	6.65636
H	86	0.24829	0.00000	0.75058	0.00113	0.75171
H	87	0.23138	0.00000	0.76772	0.00090	0.76862
H	88	0.23512	0.00000	0.76396	0.00092	0.76488

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.86)2p(2.98)3p(0.02)
C	2	[core]2S(0.98)2p(3.23)3p(0.01)
C	3	[core]2S(0.99)2p(3.17)3p(0.01)
C	4	[core]2S(0.99)2p(3.22)3p(0.01)
C	5	[core]2S(0.94)2p(3.01)3p(0.01)
C	6	[core]2S(0.79)2p(2.70)3p(0.03)
C	7	[core]2S(0.78)2p(2.88)3p(0.03)
H	8	1S(0.75)
H	9	1S(0.75)
H	10	1S(0.74)
H	11	1S(0.75)
C	12	[core]2S(0.79)2p(2.64)3p(0.02)
C	13	[core]2S(0.86)2p(2.94)3p(0.02)
C	14	[core]2S(0.98)2p(3.21)3p(0.01)
C	15	[core]2S(1.00)2p(3.12)3p(0.01)
H	16	1S(0.76)

C 17 [core]2S(0.95)2p(2.91)3p(0.01)
C 18 [core]2S(1.00)2p(3.18)3p(0.01)
H 19 1S(0.74)
H 20 1S(0.74)
C 21 [core]2S(0.89)2p(3.23)3p(0.02)
C 22 [core]2S(0.97)2p(3.19)3p(0.01)
C 23 [core]2S(0.97)2p(3.22)3p(0.01)
C 24 [core]2S(0.97)2p(3.22)3p(0.01)
H 25 1S(0.76)
C 26 [core]2S(0.97)2p(3.22)3p(0.01)
C 27 [core]2S(0.92)2p(3.04)3p(0.02)
H 28 1S(0.77)
H 29 1S(0.77)
N 30 [core]2S(1.22)2p(4.17)3p(0.01)
N 31 [core]2S(1.34)2p(4.16)3p(0.02)
N 32 [core]2S(1.30)2p(4.25)3p(0.02)
N 33 [core]2S(1.32)2p(4.44)3p(0.01)
H 34 1S(0.56)
H 35 1S(0.55)
N 36 [core]2S(1.33)2p(4.13)3p(0.02)
Pd 37 [core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)
H 38 1S(0.74)
C 39 [core]2S(0.86)2p(2.98)3p(0.02)
C 40 [core]2S(0.98)2p(3.23)3p(0.01)
C 41 [core]2S(0.99)2p(3.17)3p(0.01)
C 42 [core]2S(0.99)2p(3.22)3p(0.01)
C 43 [core]2S(0.94)2p(3.01)3p(0.01)
C 44 [core]2S(0.79)2p(2.70)3p(0.03)
C 45 [core]2S(0.78)2p(2.88)3p(0.03)
H 46 1S(0.75)
H 47 1S(0.75)
H 48 1S(0.74)
H 49 1S(0.75)
C 50 [core]2S(0.79)2p(2.64)3p(0.02)
C 51 [core]2S(0.86)2p(2.94)3p(0.02)
C 52 [core]2S(0.98)2p(3.21)3p(0.01)
C 53 [core]2S(1.00)2p(3.12)3p(0.01)
H 54 1S(0.76)
C 55 [core]2S(0.95)2p(2.91)3p(0.01)
C 56 [core]2S(1.00)2p(3.18)3p(0.01)
H 57 1S(0.74)
H 58 1S(0.74)
C 59 [core]2S(0.89)2p(3.23)3p(0.02)
C 60 [core]2S(0.97)2p(3.19)3p(0.01)
C 61 [core]2S(0.97)2p(3.22)3p(0.01)
C 62 [core]2S(0.97)2p(3.22)3p(0.01)
H 63 1S(0.76)

C	64	[core]2S(0.97)2p(3.22)3p(0.01)
C	65	[core]2S(0.92)2p(3.04)3p(0.02)
H	66	1S(0.77)
H	67	1S(0.77)
N	68	[core]2S(1.22)2p(4.17)3p(0.01)
N	69	[core]2S(1.34)2p(4.16)3p(0.02)
N	70	[core]2S(1.30)2p(4.25)3p(0.02)
N	71	[core]2S(1.32)2p(4.44)3p(0.01)
H	72	1S(0.56)
H	73	1S(0.55)
N	74	[core]2S(1.33)2p(4.13)3p(0.02)
Pd	75	[core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)
H	76	1S(0.74)
Cl	77	[core]3S(1.90)3p(5.54)
Cl	78	[core]3S(1.90)3p(5.54)
H	79	1S(0.78)
H	80	1S(0.78)
C	81	[core]2S(1.10)2p(3.55)3p(0.01)
H	82	1S(0.75)
H	83	1S(0.77)
H	84	1S(0.76)
C	85	[core]2S(1.10)2p(3.55)3p(0.01)
H	86	1S(0.75)
H	87	1S(0.77)
H	88	1S(0.76)

Summary of natural population analysis of complex 5:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.14198	1.99893	3.83530	0.02379	5.85802
C	2	-0.22328	1.99907	4.20874	0.01547	6.22328
C	3	-0.18406	1.99918	4.17013	0.01475	6.18406
C	4	-0.23392	1.99918	4.22044	0.01429	6.23392
C	5	0.05925	1.99910	3.92394	0.01772	5.94075
C	6	0.48376	1.99893	3.48421	0.03309	5.51624
C	7	0.31717	1.99880	3.65390	0.03013	5.68283
H	8	0.24614	0.00000	0.75298	0.00089	0.75386
H	9	0.24510	0.00000	0.75416	0.00073	0.75490
H	10	0.25192	0.00000	0.74740	0.00067	0.74808
H	11	0.24703	0.00000	0.75158	0.00139	0.75297
C	12	0.54689	1.99892	3.43297	0.02122	5.45311
C	13	0.18382	1.99891	3.79344	0.02383	5.81618
C	14	-0.20425	1.99908	4.19058	0.01458	6.20425
C	15	-0.13363	1.99917	4.12097	0.01349	6.13363

H	16	0.23891	0.00000	0.76018	0.00090	0.76109
C	17	0.12503	1.99914	3.86022	0.01561	5.87497
C	18	-0.19923	1.99918	4.18592	0.01413	6.19923
H	19	0.25641	0.00000	0.74278	0.00081	0.74359
H	20	0.25944	0.00000	0.73982	0.00073	0.74056
C	21	-0.17402	1.99892	4.15098	0.02413	6.17402
C	22	-0.16604	1.99913	4.15157	0.01535	6.16604
C	23	0.34780	1.99874	3.63405	0.01941	5.65220
C	24	-0.22016	1.99915	4.20672	0.01430	6.22016
H	25	0.24546	0.00000	0.75327	0.00127	0.75454
C	26	-0.29057	1.99907	4.27757	0.01393	6.29057
C	27	-0.16114	1.99917	4.14824	0.01373	6.16114
H	28	0.23731	0.00000	0.76184	0.00085	0.76269
H	29	0.23466	0.00000	0.76433	0.00102	0.76534
N	30	-0.38587	1.99927	5.37730	0.00931	7.38587
N	31	-0.51379	1.99932	5.49429	0.02017	7.51379
N	32	-0.57205	1.99932	5.55094	0.02179	7.57205
N	33	-0.78378	1.99946	5.77259	0.01173	7.78378
H	34	0.43545	0.00000	0.56370	0.00085	0.56455
H	35	0.44937	0.00000	0.54883	0.00180	0.55063
N	36	-0.47753	1.99937	5.45969	0.01847	7.47753
Pd	37	0.53500	35.98828	9.46671	0.01001	45.46500
H	38	0.25868	0.00000	0.73962	0.00169	0.74132
C	39	0.14195	1.99893	3.83533	0.02379	5.85805
C	40	-0.22330	1.99907	4.20875	0.01547	6.22330
C	41	-0.18404	1.99918	4.17012	0.01475	6.18404
C	42	-0.23391	1.99918	4.22044	0.01429	6.23391
C	43	0.05924	1.99910	3.92394	0.01772	5.94076
C	44	0.48377	1.99893	3.48420	0.03309	5.51623
C	45	0.31717	1.99880	3.65391	0.03013	5.68283
H	46	0.24614	0.00000	0.75298	0.00089	0.75386
H	47	0.24510	0.00000	0.75416	0.00073	0.75490
H	48	0.25192	0.00000	0.74740	0.00067	0.74808
H	49	0.24703	0.00000	0.75158	0.00139	0.75297
C	50	0.54688	1.99892	3.43298	0.02122	5.45312
C	51	0.18382	1.99891	3.79344	0.02383	5.81618
C	52	-0.20424	1.99908	4.19057	0.01458	6.20424
C	53	-0.13363	1.99917	4.12097	0.01349	6.13363
H	54	0.23891	0.00000	0.76019	0.00090	0.76109
C	55	0.12503	1.99914	3.86022	0.01561	5.87497
C	56	-0.19922	1.99918	4.18591	0.01413	6.19922
H	57	0.25641	0.00000	0.74278	0.00081	0.74359
H	58	0.25944	0.00000	0.73982	0.00073	0.74056

C	59	-0.17403	1.99892	4.15098	0.02413	6.17403
C	60	-0.16604	1.99913	4.15156	0.01535	6.16604
C	61	0.34781	1.99874	3.63404	0.01941	5.65219
C	62	-0.22017	1.99915	4.20672	0.01430	6.22017
H	63	0.24547	0.00000	0.75327	0.00127	0.75453
C	64	-0.29058	1.99907	4.27759	0.01393	6.29058
C	65	-0.16114	1.99917	4.14824	0.01373	6.16114
H	66	0.23731	0.00000	0.76184	0.00085	0.76269
H	67	0.23465	0.00000	0.76433	0.00102	0.76535
N	68	-0.38587	1.99927	5.37729	0.00931	7.38587
N	69	-0.51379	1.99932	5.49429	0.02017	7.51379
N	70	-0.57205	1.99932	5.55094	0.02179	7.57205
N	71	-0.78379	1.99946	5.77259	0.01173	7.78379
H	72	0.43546	0.00000	0.56369	0.00085	0.56454
H	73	0.44937	0.00000	0.54883	0.00180	0.55063
N	74	-0.47752	1.99937	5.45969	0.01847	7.47752
Pd	75	0.53501	35.98828	9.46670	0.01001	45.46499
H	76	0.25868	0.00000	0.73963	0.00169	0.74132
Cl	77	-0.44328	10.00000	7.44267	0.00061	17.44328
Cl	78	-0.44332	10.00000	7.44271	0.00061	17.44332
H	79	0.23829	0.00000	0.76083	0.00088	0.76171
H	80	0.23829	0.00000	0.76083	0.00088	0.76171
C	81	-0.25982	1.99922	4.25244	0.00817	6.25982
H	82	0.22115	0.00000	0.77821	0.00064	0.77885
H	83	0.20052	0.00000	0.79796	0.00152	0.79948
H	84	0.20474	0.00000	0.79384	0.00142	0.79526
C	85	-0.25982	1.99922	4.25244	0.00817	6.25982
H	86	0.22115	0.00000	0.77821	0.00064	0.77885
H	87	0.20052	0.00000	0.79795	0.00152	0.79948
H	88	0.20473	0.00000	0.79385	0.00142	0.79527
O	89	-0.58481	1.99982	6.57561	0.00939	8.58481
O	90	-0.58483	1.99982	6.57562	0.00939	8.58483

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.86)2p(2.98)3p(0.02)
C	2	[core]2S(0.97)2p(3.23)3p(0.01)
C	3	[core]2S(0.99)2p(3.18)3p(0.01)
C	4	[core]2S(0.99)2p(3.23)3p(0.01)
C	5	[core]2S(0.94)2p(2.99)3p(0.02)
C	6	[core]2S(0.78)2p(2.70)3p(0.03)
C	7	[core]2S(0.77)2p(2.88)3p(0.03)
H	8	1S(0.75)

	H 9	1S(0.75)
	H 10	1S(0.75)
	H 11	1S(0.75)
C 12	[core]2S(0.79)2p(2.64)3p(0.02)	
C 13	[core]2S(0.86)2p(2.94)3p(0.02)	
C 14	[core]2S(0.98)2p(3.21)3p(0.01)	
C 15	[core]2S(1.00)2p(3.12)3p(0.01)	
	H 16	1S(0.76)
C 17	[core]2S(0.95)2p(2.91)3p(0.01)	
C 18	[core]2S(1.00)2p(3.18)3p(0.01)	
	H 19	1S(0.74)
	H 20	1S(0.74)
C 21	[core]2S(0.89)2p(3.26)3p(0.02)	
C 22	[core]2S(0.97)2p(3.18)3p(0.01)	
C 23	[core]2S(0.84)2p(2.79)3p(0.02)	
C 24	[core]2S(0.98)2p(3.23)3p(0.01)	
	H 25	1S(0.75)
C 26	[core]2S(0.98)2p(3.30)3p(0.01)	
C 27	[core]2S(0.98)2p(3.16)3p(0.01)	
	H 28	1S(0.76)
	H 29	1S(0.76)
N 30	[core]2S(1.22)2p(4.16)3p(0.01)	
N 31	[core]2S(1.34)2p(4.16)3p(0.02)	
N 32	[core]2S(1.30)2p(4.25)3p(0.02)	
N 33	[core]2S(1.32)2p(4.45)3p(0.01)	
	H 34	1S(0.56)
	H 35	1S(0.55)
N 36	[core]2S(1.33)2p(4.13)3p(0.02)	
Pd 37	[core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)	
	H 38	1S(0.74)
C 39	[core]2S(0.86)2p(2.98)3p(0.02)	
C 40	[core]2S(0.97)2p(3.23)3p(0.01)	
C 41	[core]2S(0.99)2p(3.18)3p(0.01)	
C 42	[core]2S(0.99)2p(3.23)3p(0.01)	
C 43	[core]2S(0.94)2p(2.99)3p(0.02)	
C 44	[core]2S(0.78)2p(2.70)3p(0.03)	
C 45	[core]2S(0.77)2p(2.88)3p(0.03)	
	H 46	1S(0.75)
	H 47	1S(0.75)
	H 48	1S(0.75)
	H 49	1S(0.75)
C 50	[core]2S(0.79)2p(2.64)3p(0.02)	
C 51	[core]2S(0.86)2p(2.94)3p(0.02)	

C 52 [core]2S(0.98)2p(3.21)3p(0.01)
C 53 [core]2S(1.00)2p(3.12)3p(0.01)
H 54 1S(0.76)
C 55 [core]2S(0.95)2p(2.91)3p(0.01)
C 56 [core]2S(1.00)2p(3.18)3p(0.01)
H 57 1S(0.74)
H 58 1S(0.74)
C 59 [core]2S(0.89)2p(3.26)3p(0.02)
C 60 [core]2S(0.97)2p(3.18)3p(0.01)
C 61 [core]2S(0.84)2p(2.79)3p(0.02)
C 62 [core]2S(0.98)2p(3.23)3p(0.01)
H 63 1S(0.75)
C 64 [core]2S(0.98)2p(3.30)3p(0.01)
C 65 [core]2S(0.98)2p(3.16)3p(0.01)
H 66 1S(0.76)
H 67 1S(0.76)
N 68 [core]2S(1.22)2p(4.16)3p(0.01)
N 69 [core]2S(1.34)2p(4.16)3p(0.02)
N 70 [core]2S(1.30)2p(4.25)3p(0.02)
N 71 [core]2S(1.32)2p(4.45)3p(0.01)
H 72 1S(0.56)
H 73 1S(0.55)
N 74 [core]2S(1.33)2p(4.13)3p(0.02)
Pd 75 [core]5S(0.32)4d(8.86)5p(0.28)5d(0.01)
H 76 1S(0.74)
Cl 77 [core]3S(1.90)3p(5.54)
Cl 78 [core]3S(1.90)3p(5.54)
H 79 1S(0.76)
H 80 1S(0.76)
C 81 [core]2S(1.10)2p(3.15)3p(0.01)
H 82 1S(0.78)
H 83 1S(0.80)
H 84 1S(0.79)
C 85 [core]2S(1.10)2p(3.15)3p(0.01)
H 86 1S(0.78)
H 87 1S(0.80)
H 88 1S(0.79)
O 89 [core]2S(1.64)2p(4.94)3p(0.01)
O 90 [core]2S(1.64)2p(4.94)3p(0.01)

Cartesian coordinates

Cartesian coordinates of **L1H**:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.115827	1.933213	0.075208
2	6	2.434157	2.638531	0.193202
3	6	2.022948	3.912749	0.423305
4	6	0.632284	4.242288	0.477918
5	6	-0.30289	3.256746	0.311934
6	6	-0.53222	0.703418	-0.10301
7	6	1.609769	0.287148	-0.2192
8	1	3.468677	2.331697	0.157341
9	1	2.772627	4.679227	0.573097
10	1	0.331288	5.266197	0.659578
11	1	-1.36791	3.443446	0.360597
12	6	2.901447	-0.39119	-0.40536
13	6	3.809442	0.059343	-1.36899
14	6	5.032938	-0.57349	-1.5766
15	1	3.535844	0.9103	-1.98287
16	6	4.471975	-2.16518	0.152934
17	6	5.35685	-1.68837	-0.81352
18	1	5.713813	-0.20669	-2.3352
19	1	4.74569	-3.03139	0.739584
20	1	6.301229	-2.1991	-0.96453
21	6	-2.49022	-0.56766	-0.20024
22	6	-3.98649	-0.59318	-0.15716
23	6	-4.70285	-1.53323	-0.91204
24	6	-6.09223	-1.52572	-0.85781
25	1	-4.17602	-2.23012	-1.55189
26	6	-5.92646	0.30944	0.6593
27	6	-6.72519	-0.58618	-0.05214
28	1	-6.668	-2.2347	-1.44247
29	1	-6.38355	1.059773	1.299817
30	1	-7.80505	-0.54077	0.024817
31	7	0.409396	-0.27594	-0.28022
32	7	-1.89736	0.574244	-0.0876
33	7	-4.59584	0.316223	0.616952
34	7	-1.88086	-1.77781	-0.4347
35	1	-2.35846	-2.61098	-0.12946
36	1	-0.8645	-1.7698	-0.39186
37	7	1.489841	1.644688	0.000206
38	6	3.248654	-1.52451	0.367714
39	8	2.348231	-1.91146	1.307548
40	6	2.650485	-3.02822	2.130763

41	1	3.55627	-2.85892	2.723808
42	1	1.79852	-3.13839	2.799307
43	1	2.768095	-3.94354	1.540167

Cartesian coordinates of **L2H**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.455514	1.940009	0.108573
2	6	-1.77229	2.88449	0.238663
3	6	-1.22815	4.128117	0.293922
4	6	0.186913	4.321337	0.232011
5	6	1.011771	3.232236	0.150437
6	6	0.979894	0.641331	0.070176
7	6	-1.19889	0.425101	0.065649
8	1	-2.83051	2.688582	0.309637
9	1	-1.89179	4.977285	0.396422
10	1	0.593617	5.323973	0.265329
11	1	2.09086	3.311994	0.124147
12	6	-2.52573	-0.19319	0.059967
13	6	-3.61771	0.337393	-0.63625
14	6	-4.85858	-0.29981	-0.64285
15	1	-3.50257	1.24145	-1.22198
16	6	-3.93532	-2.05597	0.733321
17	6	-5.02563	-1.50169	0.048042
18	1	-5.67323	0.14141	-1.20102
19	1	-4.0807	-2.99112	1.260521
20	6	2.815217	-0.80105	-0.06611
21	6	4.304181	-0.95281	-0.10122
22	6	4.916601	-2.08368	0.4576
23	6	6.302425	-2.19062	0.416541
24	1	4.315774	-2.84297	0.942422
25	6	6.334842	-0.085	-0.70723
26	6	7.034506	-1.17161	-0.18169
27	1	6.799522	-3.04988	0.852979
28	1	6.871316	0.732559	-1.1825
29	1	8.11581	-1.20936	-0.23986
30	7	-0.05489	-0.25564	0.052733
31	7	2.32688	0.389831	0.038378
32	7	5.009257	0.032941	-0.67439
33	7	2.096834	-1.97395	-0.07635
34	1	2.507016	-2.7695	-0.53992
35	1	1.088081	-1.86446	-0.1353
36	7	-0.94291	1.781456	0.110275

37	6	-2.71184	-1.41344	0.737769
38	8	-6.18858	-2.20785	0.112269
39	1	-1.87441	-1.84507	1.27153
40	6	-7.32812	-1.70121	-0.56817
41	1	-7.15422	-1.63311	-1.64789
42	1	-8.12895	-2.41368	-0.37779
43	1	-7.6208	-0.71743	-0.18434

Cartesian coordinates of **L3H**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.170477	1.88942	-0.18701
2	6	2.494177	2.568355	-0.32518
3	6	2.094511	3.841856	-0.57961
4	6	0.708087	4.18511	-0.63299
5	6	-0.23625	3.212107	-0.44489
6	6	-0.49386	0.670351	0.016313
7	6	1.642661	0.233553	0.13788
8	1	3.526214	2.253415	-0.29241
9	1	2.851536	4.596535	-0.75049
10	1	0.416862	5.208434	-0.8324
11	1	-1.29967	3.408273	-0.48956
12	6	2.919118	-0.46049	0.353074
13	6	3.835488	0.040403	1.2949
14	6	5.041569	-0.59698	1.555837
15	1	3.571791	0.933534	1.849529
16	6	4.474423	-2.29643	-0.05301
17	6	5.361585	-1.77261	0.881248
18	1	5.720215	-0.18627	2.294104
19	1	4.71075	-3.2053	-0.5911
20	1	6.296154	-2.28447	1.078484
21	6	-2.46968	-0.55902	0.220356
22	6	-3.96737	-0.55805	0.210694
23	6	-4.67518	-1.65952	-0.29056
24	6	-6.06527	-1.62309	-0.29451
25	1	-4.14151	-2.50902	-0.69835
26	6	-5.91471	0.551643	0.678241
27	6	-6.70606	-0.49459	0.203629
28	1	-6.63487	-2.45736	-0.68871
29	1	-6.37819	1.451472	1.075075
30	1	-7.78675	-0.41908	0.223538
31	7	0.435425	-0.3158	0.206341
32	7	-1.86001	0.56326	0.022126

33	7	-4.5834	0.53298	0.686686
34	7	-1.87675	-1.78661	0.369763
35	1	-2.38869	-2.50968	0.848888
36	1	-0.86335	-1.78652	0.444621
37	7	1.540669	1.58879	-0.10404
38	6	3.272844	-1.6451	-0.31664
39	17	2.228735	-2.33729	-1.54729

Cartesian coordinates of **L4H**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.02428	1.870673	-0.1103
2	6	2.248143	2.702968	-0.21531
3	6	1.766349	3.970595	-0.3002
4	6	0.362003	4.23336	-0.2676
5	6	-0.51642	3.187078	-0.18347
6	6	-0.61333	0.599582	-0.06104
7	6	1.551379	0.276972	-0.01599
8	1	3.296604	2.455252	-0.26361
9	1	2.47258	4.784532	-0.40354
10	1	0.005371	5.253806	-0.32493
11	1	-1.59065	3.319204	-0.17839
12	6	2.84508	-0.40688	0.023966
13	6	3.954952	0.090296	0.723129
14	6	5.153173	-0.61745	0.754476
15	1	3.876291	1.012124	1.286778
16	6	4.17371	-2.34929	-0.57631
17	6	5.290734	-1.84464	0.101925
18	1	5.991721	-0.21267	1.312171
19	1	4.246258	-3.30592	-1.08447
20	6	-2.52011	-0.74711	0.068981
21	6	-4.01522	-0.82458	0.080944
22	6	-4.67372	-1.93272	-0.4708
23	6	-6.06365	-1.97043	-0.45153
24	1	-4.10359	-2.72855	-0.93364
25	6	-6.00965	0.152178	0.639133
26	6	-6.75372	-0.907	0.118602
27	1	-6.59574	-2.81101	-0.88303
28	1	-6.51246	1.002785	1.092642
29	1	-7.83635	-0.89047	0.159163
30	7	0.374516	-0.34624	-0.0134
31	7	-1.97152	0.41615	-0.04825
32	7	-4.67946	0.203996	0.626779

33	7	-1.86123	-1.95323	0.112837
34	1	-2.3187	-2.72009	0.580389
35	1	-0.84928	-1.8936	0.18602
36	7	1.363741	1.643947	-0.08435
37	6	2.97648	-1.64989	-0.61749
38	1	2.123519	-2.05387	-1.14855
39	6	6.598504	-2.5971	0.112141
40	1	6.439206	-3.67178	0.233357
41	1	7.143072	-2.45395	-0.82777
42	1	7.247339	-2.2579	0.922444

Cartesian coordinates of **L5H**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.27593	2.073370	-0.10434
2	6	0.83291	3.257068	-0.21556
3	6	0.154402	4.432618	-0.28397
4	6	-1.27269	4.468264	-0.23935
5	6	-1.97246	3.294255	-0.16102
6	6	-1.65752	0.72362	-0.06584
7	6	0.530446	0.748191	-0.0368
8	1	1.906847	3.182357	-0.27724
9	1	0.721431	5.349264	-0.38433
10	1	-1.78769	5.41926	-0.28402
11	1	-3.05388	3.252555	-0.14861
12	6	1.912132	0.270766	-0.00865
13	6	2.943496	0.940216	0.669541
14	6	4.238413	0.430633	0.693788
15	1	2.735897	1.846153	1.225155
16	6	3.505536	-1.46516	-0.62009
17	6	4.511724	-0.76707	0.043258
18	1	5.020605	0.954052	1.228103
19	1	3.726972	-2.39922	-1.12002
20	6	-3.33003	-0.9045	0.066534
21	6	-4.79513	-1.21369	0.084304
22	6	-5.27674	-2.40557	-0.47477
23	6	-6.64408	-2.65813	-0.44946
24	1	-4.59343	-3.09987	-0.94776
25	6	-6.91276	-0.56189	0.660838
26	6	-7.48672	-1.71919	0.133841
27	1	-7.0423	-3.5671	-0.88642
28	1	-7.5384	0.196592	1.124667
29	1	-8.55857	-1.8708	0.179456

30	7	-0.53389	-0.05398	-0.0351
31	7	-2.9699	0.330767	-0.04842
32	7	-5.60665	-0.3047	0.642528
33	7	-2.49186	-1.99185	0.106264
34	1	-2.82494	-2.82744	0.56066
35	1	-1.50065	-1.77985	0.17289
36	7	0.129836	2.069361	-0.08881
37	6	2.218226	-0.9458	-0.642
38	1	1.429545	-1.47784	-1.15863
39	35	6.295044	-1.47181	0.067979

Cartesian coordinates of **1**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.40473	0.600031	2.522179
2	6	-1.94556	1.70284	3.246069
3	6	-3.17111	1.558657	3.868126
4	6	-3.89041	0.312547	3.779012
5	6	-3.38747	-0.74195	3.058802
6	6	-1.43871	-1.52409	1.666265
7	6	-0.21445	0.346392	1.828941
8	1	-1.38317	2.62902	3.299884
9	1	-3.59629	2.378383	4.43855
10	1	-4.83953	0.193259	4.289486
11	1	-3.88083	-1.69754	2.955526
12	6	1.759009	1.552213	2.469189
13	6	2.847147	2.460802	2.017464
14	6	3.788419	3.063738	2.861639
15	6	4.783092	3.891162	2.302841
16	1	3.757206	2.918797	3.936664
17	6	3.828795	3.467644	0.114216
18	6	4.804978	4.090834	0.913739
19	1	5.518508	4.368546	2.942587
20	1	5.554743	4.718944	0.445362
21	6	-1.85571	-2.90863	1.388626
22	6	-1.02653	-3.98835	1.770367
23	6	-3.08587	-3.18736	0.731336
24	6	-1.40881	-5.31512	1.512441
25	1	-0.09508	-3.78233	2.289582
26	6	-3.47205	-4.51638	0.47489
27	6	-2.63164	-5.57419	0.867583
28	1	-0.76895	-6.13397	1.826007

29	1	-4.41207	-4.73654	-0.01928
30	7	-2.15533	-0.60114	2.421041
31	7	-0.2677	-0.9402	1.312871
32	7	0.861304	1.212682	1.544289
33	7	1.734607	1.105727	3.745565
34	1	2.488478	1.299731	4.390328
35	1	1.090777	0.366562	4.009226
36	7	2.875432	2.676756	0.66068
37	46	1.33914	1.800497	-0.37635
38	1	3.793079	3.586104	-0.96281
39	6	-1.40453	-0.59962	-2.52256
40	6	-1.94554	-1.70228	-3.24654
41	6	-3.17097	-1.55778	-3.86877
42	6	-3.88997	-0.3115	-3.77971
43	6	-3.38689	0.742829	-3.05935
44	6	-1.43816	1.524452	-1.66648
45	6	-0.21431	-0.34633	-1.8291
46	1	-1.38338	-2.62861	-3.30029
47	1	-3.59626	-2.37738	-4.43927
48	1	-4.83899	-0.19195	-4.29032
49	1	-3.88004	1.698524	-2.95612
50	6	1.758821	-1.55276	-2.46916
51	6	2.84672	-2.46153	-2.01727
52	6	3.788118	-3.06454	-2.86125
53	6	4.782516	-3.89216	-2.30228
54	1	3.757241	-2.91948	-3.93627
55	6	3.827734	-3.4687	-0.11386
56	6	4.804007	-4.092	-0.91319
57	1	5.518046	-4.36956	-2.94188
58	1	5.553534	-4.7203	-0.44469
59	6	-1.85489	2.909051	-1.38877
60	6	-1.02552	3.988627	-1.77055
61	6	-3.08493	3.188038	-0.73133
62	6	-1.4075	5.315466	-1.51254
63	1	-0.09418	3.782445	-2.2899
64	6	-3.47079	4.517116	-0.47478
65	6	-2.6302	5.574773	-0.86754
66	1	-0.76748	6.134194	-1.82612
67	1	-4.41068	4.737463	0.019535
68	7	-2.15489	0.601698	-2.42141

69	7	-0.2673	0.940302	-1.31305
70	7	0.861193	-1.21289	-1.5443
71	7	1.73447	-1.10651	-3.74562
72	1	2.488238	-1.30081	-4.39041
73	1	1.090532	-0.36752	-4.00952
74	7	2.874673	-2.67758	-0.6605
75	46	1.338602	-1.80082	0.376381
76	1	3.791732	-3.58723	0.963147
77	17	2.185107	2.325448	-2.56272
78	17	2.184239	-2.32581	2.562916
79	1	-2.93792	6.598746	-0.67383
80	1	-2.93959	-6.59811	0.673968
81	6	-5.10568	2.276999	0.346931
82	1	-5.48716	1.273817	0.542441
83	1	-4.93622	2.799799	1.296124
84	1	-5.82202	2.83746	-0.26667
85	6	-5.10675	-2.27581	-0.34637
86	1	-5.48824	-1.27254	-0.54142
87	1	-4.9377	-2.79831	-1.2958
88	1	-5.8229	-2.83643	0.267309
89	8	-3.84409	2.073923	-0.36829
90	8	-3.84488	-2.07306	0.368446

Cartesian coordinates of **2**:

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	6	-0.66534	-1.42861	2.467692
2	6	-1.80486	-1.90953	3.178951
3	6	-1.75588	-3.16416	3.754318
4	6	-0.56492	-3.97073	3.642368
5	6	0.524566	-3.52634	2.937047
6	6	1.442514	-1.60124	1.577761
7	6	-0.32466	-0.23894	1.813266
8	1	-2.68509	-1.28014	3.255519
9	1	-2.60811	-3.54932	4.30461
10	1	-0.51573	-4.94028	4.125298
11	1	1.448342	-4.07982	2.834105
12	6	-1.34528	1.826346	2.491651
13	6	-2.22546	2.955099	2.082734
14	6	-2.7268	3.934109	2.949859
15	6	-3.54749	4.956355	2.431903

16	1	-2.50944	3.91199	4.012874
17	6	-3.315	3.955483	0.235371
18	6	-3.84108	4.967883	1.059457
19	1	-3.94814	5.720574	3.090268
20	1	-4.46811	5.737357	0.622647
21	6	2.751195	-2.1627	1.218608
22	6	3.947157	-1.46727	1.507931
23	6	2.834991	-3.42808	0.575976
24	6	5.196934	-2.01423	1.176267
25	1	3.903331	-0.51005	2.019965
26	6	4.071999	-3.9775	0.239359
27	6	5.26532	-3.27582	0.541713
28	1	6.098834	-1.46673	1.428461
29	1	4.151177	-4.94247	-0.25098
30	7	0.471495	-2.27024	2.323986
31	7	0.946983	-0.37725	1.272158
32	7	-1.12143	0.897601	1.561516
33	7	-0.81234	1.794887	3.733231
34	1	-0.93535	2.55811	4.384526
35	1	-0.08314	1.123191	3.953599
36	7	-2.53094	2.975449	0.743072
37	46	-1.77803	1.399263	-0.33019
38	1	-3.50589	3.912329	-0.83095
39	6	0.47101	-1.43201	-2.52457
40	6	1.552855	-2.022	-3.24361
41	6	1.363433	-3.24466	-3.85703
42	6	0.083676	-3.90603	-3.77969
43	6	-0.9522	-3.35865	-3.06611
44	6	-1.64731	-1.38412	-1.64216
45	6	0.267309	-0.2297	-1.83776
46	1	2.501725	-1.49879	-3.29464
47	1	2.170936	-3.71258	-4.41051
48	1	-0.07577	-4.84606	-4.29602
49	1	-1.9365	-3.80058	-2.99154
50	6	1.51669	1.721765	-2.46715
51	6	2.521586	2.731188	-2.03394
52	6	3.124934	3.673094	-2.877
53	6	4.056203	4.582746	-2.3368
54	1	2.900761	3.706878	-3.93827
55	6	3.723623	3.551192	-0.16758

56	6	4.355115	4.522383	-0.96671
57	1	4.535513	5.317082	-2.97635
58	1	5.064442	5.205856	-0.51306
59	6	-3.0158	-1.79125	-1.30043
60	6	-4.10694	-0.90353	-1.50112
61	6	-3.27624	-3.07511	-0.76505
62	6	-5.40727	-1.29382	-1.17948
63	1	-3.9344	0.073785	-1.94207
64	6	-4.58112	-3.47747	-0.44185
65	6	-5.65756	-2.58337	-0.65109
66	1	-6.25157	-0.63283	-1.34688
67	1	-4.74951	-4.46851	-0.03383
68	7	-0.75729	-2.13919	-2.40852
69	7	-1.01339	-0.23419	-1.30128
70	7	1.188123	0.802092	-1.55907
71	7	0.982007	1.783209	-3.70652
72	1	1.192705	2.542318	-4.33992
73	1	0.174199	1.212098	-3.93688
74	7	2.833554	2.678894	-0.69668
75	46	1.904096	1.173888	0.340307
76	1	3.912008	3.456861	0.895917
77	17	-2.36922	2.259318	-2.49337
78	17	2.614803	1.887079	2.520829
79	1	-2.4568	-3.76461	-0.57208
80	1	1.929242	-3.97429	0.320505
81	6	7.726723	-3.30766	0.497335
82	1	7.845148	-2.34147	-0.00975
83	1	7.840364	-3.18602	1.581757
84	1	8.467759	-4.01487	0.124218
85	6	-7.36068	-4.19585	0.100172
86	1	-6.90609	-4.4075	1.076683
87	1	-8.4458	-4.15856	0.198219
88	1	-7.07922	-4.96747	-0.62743
89	8	6.430554	-3.91202	0.174564
90	8	-6.97794	-2.86446	-0.37796

Cartesian coordinates of **3**:

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	6	-0.45844	-1.39494	2.627282
2	6	-1.51611	-1.90391	3.435736

3	6	-1.34282	-3.11315	4.081567
4	6	-0.11161	-3.84642	3.936417
5	6	0.903433	-3.37055	3.144925
6	6	1.605072	-1.46904	1.644456
7	6	-0.24803	-0.23504	1.866598
8	1	-2.43646	-1.33671	3.525022
9	1	-2.13329	-3.52185	4.702452
10	1	0.025306	-4.79001	4.452381
11	1	1.847165	-3.87835	2.998361
12	6	-1.42145	1.744672	2.539186
13	6	-2.36639	2.817879	2.128706
14	6	-2.92824	3.764131	2.995409
15	6	-3.80032	4.741465	2.47508
16	1	-2.71817	3.750212	4.059985
17	6	-3.49881	3.761807	0.277528
18	6	-4.08448	4.741627	1.100651
19	1	-4.24679	5.480226	3.133021
20	1	-4.74909	5.477503	0.661534
21	6	2.976374	-1.90949	1.317469
22	6	4.084026	-1.17192	1.805446
23	6	3.245445	-3.06555	0.550668
24	6	5.398878	-1.58871	1.539365
25	1	3.902274	-0.28057	2.398632
26	6	4.548438	-3.49806	0.279893
27	6	5.632425	-2.75257	0.78286
28	1	6.233926	-1.01565	1.930765
29	1	4.715353	-4.39484	-0.30749
30	1	6.647204	-3.08498	0.584239
31	17	1.863357	-4.03394	-0.14564
32	7	0.732353	-2.15279	2.484058
33	7	1.004783	-0.31249	1.277813
34	7	-1.12603	0.837699	1.606905
35	7	-0.90272	1.74112	3.788104
36	1	-1.07569	2.496218	4.437447
37	1	-0.14472	1.107265	4.020503
38	7	-2.66452	2.825186	0.787394
39	46	-1.82924	1.29081	-0.28366
40	1	-3.68161	3.710703	-0.78975
41	6	0.443762	-1.40072	-2.62642
42	6	1.49601	-1.92104	-3.43473

43	6	1.309944	-3.12851	-4.08032
44	6	0.07106	-3.8487	-3.93502
45	6	-0.93888	-3.36196	-3.14361
46	6	-1.62043	-1.45285	-1.64364
47	6	0.245665	-0.23859	-1.8658
48	1	2.42237	-1.3637	-3.52403
49	1	2.096068	-3.54571	-4.70108
50	1	-0.07585	-4.7909	-4.45078
51	1	-1.88787	-3.8598	-2.99683
52	6	1.440106	1.728102	-2.53943
53	6	2.396366	2.791444	-2.12956
54	6	2.968068	3.731364	-2.99674
55	6	3.85051	4.699621	-2.47695
56	1	2.757715	3.719265	-4.06128
57	6	3.538938	3.724196	-0.27893
58	6	4.134876	4.69737	-1.10256
59	1	4.304653	5.43335	-3.13528
60	1	4.807328	5.426343	-0.66387
61	6	-2.99654	-1.87855	-1.31728
62	6	-4.09588	-1.12933	-1.80636
63	6	-3.27854	-3.03138	-0.5503
64	6	-5.41532	-1.53195	-1.54119
65	1	-3.90409	-0.24017	-2.39966
66	6	-4.58631	-3.44983	-0.28038
67	6	-5.66188	-2.693	-0.78448
68	1	-6.24388	-0.95011	-1.93342
69	1	-4.76325	-4.34456	0.307188
70	1	-6.6803	-3.01449	-0.58653
71	17	-1.90747	-4.01425	0.147481
72	7	-0.75494	-2.14593	-2.48302
73	7	-1.00788	-0.30275	-1.27692
74	7	1.134802	0.825029	-1.60654
75	7	0.921451	1.729207	-3.78841
76	1	1.102768	2.481764	-4.43841
77	1	0.156629	1.103428	-4.02033
78	7	2.694689	2.796261	-0.78828
79	46	1.842968	1.271639	0.283711
80	1	3.721298	3.671684	0.788354
81	17	-2.49352	2.108871	-2.4418
82	17	2.515995	2.083468	2.441455

Cartesian coordinates of **4**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.59775	-1.55367	2.495218
2	6	-1.71625	-2.0865	3.202442
3	6	-1.60359	-3.327	3.799101
4	6	-0.36771	-4.06597	3.713657
5	6	0.703375	-3.57219	3.01298
6	6	1.525416	-1.61951	1.630666
7	6	-0.31836	-0.35738	1.823392
8	1	-2.63152	-1.50701	3.258524
9	1	-2.43953	-3.75159	4.345288
10	1	-0.26974	-5.02349	4.212877
11	1	1.657847	-4.07431	2.929655
12	6	-1.46094	1.656886	2.460101
13	6	-2.40268	2.725232	2.026437
14	6	-2.96633	3.687834	2.87347
15	6	-3.841	4.651947	2.332893
16	1	-2.75542	3.696635	3.937972
17	6	-3.53453	3.629987	0.155231
18	6	-4.12456	4.623613	0.958564
19	1	-4.28969	5.402767	2.975498
20	1	-4.79137	5.348446	0.504644
21	6	2.871623	-2.10852	1.294337
22	6	4.017132	-1.32374	1.568071
23	6	3.041854	-3.37938	0.692235
24	6	5.295449	-1.80815	1.251152
25	1	3.907662	-0.3568	2.050882
26	6	4.3255	-3.85223	0.380444
27	6	5.477677	-3.08029	0.660135
28	1	6.165465	-1.1978	1.481811
29	1	4.437036	-4.82997	-0.08218
30	7	0.586867	-2.33107	2.377912
31	7	0.965286	-0.43085	1.299324
32	7	-1.17543	0.728325	1.546417
33	7	-0.9371	1.676521	3.70548
34	1	-1.1123	2.440131	4.344321
35	1	-0.16637	1.05774	3.939648
36	7	-2.69886	2.705632	0.684641
37	46	-1.84158	1.163183	-0.35824

38	1	-3.71395	3.558551	-0.91156
39	6	0.597377	-1.55393	-2.49522
40	6	1.715724	-2.08698	-3.20254
41	6	1.602758	-3.32744	-3.79923
42	6	0.366734	-4.06616	-3.71372
43	6	-0.7042	-3.57217	-3.01296
44	6	-1.52573	-1.61939	-1.63051
45	6	0.318311	-0.35766	-1.82323
46	1	2.63112	-1.50768	-3.25867
47	1	2.438577	-3.75219	-4.34548
48	1	0.268542	-5.02366	-4.21294
49	1	-1.65876	-4.0741	-2.92955
50	6	1.461469	1.656145	-2.46025
51	6	2.403286	2.724462	-2.0267
52	6	2.967148	3.686815	-2.87388
53	6	3.841834	4.650962	-2.3334
54	1	2.756378	3.695405	-3.93841
55	6	3.534977	3.629522	-0.15555
56	6	4.125213	4.622912	-0.95903
57	1	4.29068	5.401597	-2.97612
58	1	4.792025	5.347792	-0.50518
59	6	-2.872	-2.1082	-1.29408
60	6	-4.01742	-1.3233	-1.56786
61	6	-3.04235	-3.37895	-0.69185
62	6	-5.29577	-1.80751	-1.25084
63	1	-3.90782	-0.3564	-2.05073
64	6	-4.32605	-3.85163	-0.37994
65	6	-5.47813	-3.0796	-0.65969
66	1	-6.16574	-1.19707	-1.48146
67	1	-4.43766	-4.82929	0.082835
68	7	-0.58739	-2.33108	-2.37788
69	7	-0.96531	-0.4309	-1.29907
70	7	1.175541	0.727938	-1.54634
71	7	0.937934	1.675479	-3.70578
72	1	1.113335	2.438911	-4.34478
73	1	0.167277	1.056633	-3.94
74	7	2.699281	2.705136	-0.68486
75	46	1.841749	1.162982	0.358267
76	1	3.714276	3.558294	0.911279
77	17	-2.46543	1.951262	-2.53919

78	17	2.465801	1.951216	2.539112
79	1	-2.17598	-3.98947	-0.4442
80	1	2.175419	-3.9898	0.444618
81	6	-6.86594	-3.60953	-0.3637
82	1	-7.3091	-4.05809	-1.26383
83	1	-6.84881	-4.3833	0.411352
84	1	-7.54146	-2.81102	-0.03615
85	6	6.865401	-3.61039	0.363985
86	1	7.308632	-4.05916	1.263962
87	1	6.84805	-4.38401	-0.41122
88	1	7.540974	-2.81192	0.036434

Cartesian coordinates of **5**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.58298	172521 2.	515950
2	6	-1.69558	-1.69716	3.238152
3	6	-1.58016	-2.93362	3.843214
4	6	-0.34678	-3.67558	3.751965
5	6	0.719367	-3.18913	3.038456
6	6	1.530488	-1.24698	1.633856
7	6	-0.30825	0.018657	1.831191
8	1	-2.60876	-1.11492	3.300105
9	1	-2.41166	-3.35188	4.400888
10	1	-0.24607	-4.62935	4.25781
11	1	1.672307	-3.69406	2.953546
12	6	-1.4493	2.03434	2.468512
13	6	-2.39794	3.097535	2.037504
14	6	-2.96058	4.060008	2.885199
15	6	-3.84388	5.018083	2.347614
16	1	-2.74292	4.073506	3.948308
17	6	-3.54638	3.991198	0.170928
18	6	-4.13627	4.984177	0.975341
19	1	-4.29241	5.768309	2.991006
20	1	-4.80999	5.704022	0.523692
21	6	2.872202	-1.73902	1.280901
22	6	4.019515	-0.95167	1.537056
23	6	3.029159	-3.01032	0.675575
24	6	5.296788	-1.42455	1.193366
25	1	3.92013	0.012292	2.02751

26	6	4.303442	-3.48679	0.331095
27	6	5.43325	-2.68805	0.59061
28	1	6.172813	-0.8207	1.407666
29	1	4.414618	-4.46196	-0.1324
30	7	0.599408	-1.95246	2.394622
31	7	0.970155	-0.05994	1.297436
32	7	-1.16618	1.103594	1.555407
33	7	-0.91766	2.05965	3.710004
34	1	-1.09679	2.821111	4.350497
35	1	-0.14422	1.444035	3.943512
36	7	-2.70286	3.07232	0.69755
37	46	-1.84541	1.531487	-0.3466
38	1	-3.73292	3.916481	-0.89436
39	6	0.582844	-1.1727	-2.51589
40	6	1.695414	-1.6974	-3.23811
41	6	1.579919	-2.93386	-3.84317
42	6	0.346513	-3.67577	-3.75188
43	6	-0.71959	-3.18927	-3.03834
44	6	-1.53059	-1.24709	-1.63374
45	6	0.308222	0.018443	-1.83103
46	1	2.608631	-1.11523	-3.30005
47	1	2.411399	-3.35216	-4.40084
48	1	0.245749	-4.62954	-4.25771
49	1	-1.67254	-3.69418	-2.95338
50	6	1.44968	2.033769	-2.46869
51	6	2.398259	3.097051	-2.03776
52	6	2.960848	4.059491	-2.88553
53	6	3.844077	5.017671	-2.34801
54	1	2.743189	4.072919	-3.94863
55	6	3.546577	3.990987	-0.17124
56	6	4.136451	4.983913	-0.97573
57	1	4.292549	5.767881	-2.99146
58	1	4.810126	5.703839	-0.52414
59	6	-2.87233	-1.73906	-1.28077
60	6	-4.0196	-0.95162	-1.53689
61	6	-3.02936	-3.01037	-0.67547
62	6	-5.2969	-1.42442	-1.19319
63	1	-3.92015	0.012335	-2.02734
64	6	-4.30368	-3.48676	-0.33099
65	6	-5.43343	-2.68792	-0.59046

66	1	-6.17289	-0.82051	-1.40746
67	1	-4.41491	-4.46192	0.132499
68	7	-0.59956	-1.9526	-2.39452
69	7	-0.97019	-0.06011	-1.29725
70	7	1.166172	1.103383	-1.55532
71	7	0.918444	2.058671	-3.71036
72	1	1.09785	2.81985	-4.35111
73	1	0.14516	1.4429	-3.94395
74	7	2.70311	3.072024	-0.69779
75	46	1.845476	1.531462	0.3466
76	1	3.733094	3.916388	0.894065
77	17	-2.4944	2.304463	-2.52449
78	17	2.494456	2.304707	2.52442
79	1	-2.16153	-3.62603	-0.44931
80	1	2.161286	-3.62591	0.44938
81	35	-7.20823	-3.34678	-0.11509
82	35	7.208007	-3.34703	0.115284

Cartesian coordinates of **3o**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.65626	2.630967	0.798146
2	6	3.941494	-1.43424	0.833167
3	6	2.849725	-1.23497	-0.02501
4	6	2.490382	-2.26299	-0.9099
5	6	3.202138	-3.46187	-0.92313
6	6	4.302405	-3.66943	-0.07684
7	1	5.494247	-2.7648	1.471364
8	1	4.223173	-0.65253	1.524579
9	1	1.654402	-2.12048	-1.58024
10	1	2.90511	-4.24361	-1.61157
11	6	2.848328	1.235384	0.024804
12	6	3.947152	1.433639	-0.82435
13	6	2.486205	2.261767	0.910758
14	6	4.664142	2.628949	-0.78192
15	1	4.237347	0.649637	-1.50959
16	6	3.20017	3.459055	0.931307
17	1	1.650861	2.11605	1.581191
18	6	4.302738	3.668633	0.088362
19	1	5.511657	2.759212	-1.44377
20	1	2.905148	4.237079	1.624842
21	6	0.702144	-0.00071	-0.00156
22	6	-0.01933	1.007741	-0.6693

23	6	-0.01871	-1.00958	0.666218
24	6	-1.40824	1.009512	-0.66332
25	1	0.516129	1.78461	-1.19522
26	6	-1.40763	-1.01207	0.660408
27	1	0.517181	-1.78624	1.192021
28	6	-2.13805	-0.00143	-0.00134
29	1	-1.94499	1.789552	-1.1856
30	1	-1.94387	-1.7924	1.182767
31	6	5.09443	-4.95638	-0.12448
32	1	4.46541	-5.80213	-0.40671
33	1	5.907149	-4.89749	-0.85516
34	1	5.54453	-5.18337	0.843321
35	6	5.059343	4.977504	0.101675
36	1	6.105947	4.836455	-0.17271
37	1	4.630806	5.692835	-0.60721
38	1	5.032568	5.44345	1.088095
39	6	-3.56126	-0.00167	-0.00109
40	6	-4.77627	-0.00183	-0.00084
41	7	2.122457	-0.00014	-0.00148
42	6	-6.20158	-0.002	-0.00044
43	6	-6.92358	1.019971	-0.65405
44	6	-6.92297	-1.02415	0.653575
45	6	-8.31692	1.015984	-0.65117
46	1	-6.38025	1.80736	-1.15788
47	6	-8.31631	-1.02049	0.651505
48	1	-6.37916	-1.81141	1.157092
49	6	-9.01959	-0.00233	0.000375
50	1	-8.85503	1.806896	-1.15697
51	1	-8.85393	-1.81152	1.157634
52	1	-10.1014	-0.00246	0.000677

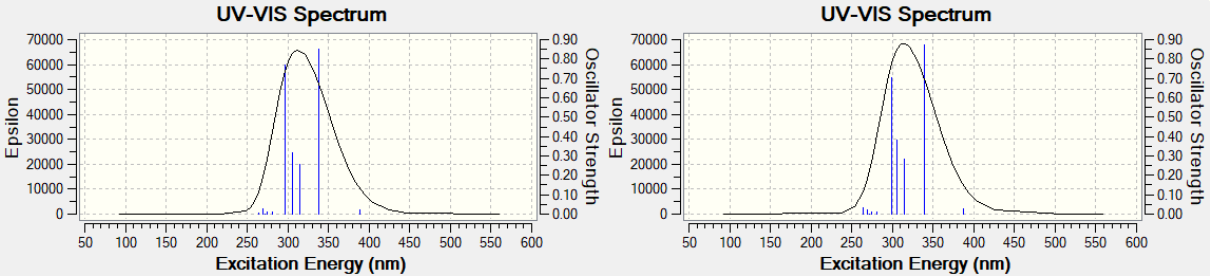
Cartesian coordinates of **3p**:

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	6	2.658488	-1.0828	-0.95040
2	6	1.695385	-0.1559	-0.50806
3	6	0.388131	-0.18171	-1.01141
4	6	0.036836	-1.15648	-1.96125
5	6	0.982854	-2.08877	-2.38767
6	6	2.287086	-2.06005	-1.89791
7	1	1.971371	0.584222	0.22813
8	1	-0.96737	-1.17537	-2.35893

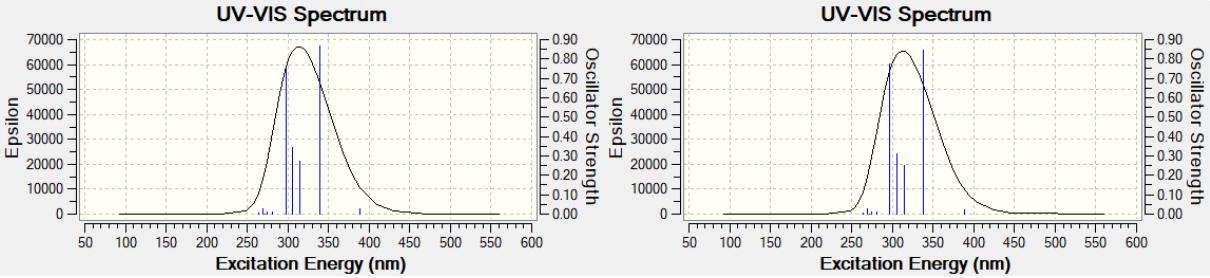
9	1	0.701721	-2.83413	-3.11987
10	6	-0.19497	2.142625	-0.3838
11	6	0.613373	2.788812	-1.33377
12	6	-0.62685	2.856779	0.746111
13	6	0.987231	4.120195	-1.14905
14	1	0.942857	2.24648	-2.20851
15	6	-0.26257	4.193065	0.914295
16	1	-1.24223	2.361885	1.483823
17	6	0.549004	4.831711	-0.02814
18	1	1.611043	4.604409	-1.88877
19	1	-0.60249	4.730396	1.789873
20	6	-1.91709	0.366434	-0.29678
21	6	-3.00195	1.167885	-0.68892
22	6	-2.1813	-0.84357	0.366018
23	6	-4.30855	0.770421	-0.41897
24	1	-2.81629	2.094092	-1.21384
25	6	-3.49178	-1.24006	0.618259
26	1	-1.35757	-1.46264	0.691933
27	6	-4.58731	-0.4434	0.236468
28	1	-5.12653	1.392766	-0.75668
29	1	-3.66649	-2.16297	1.155077
30	7	-0.57515	0.774615	-0.56496
31	6	-5.98312	-0.86705	0.514466
32	6	-6.36852	-2.2158	0.395539
33	6	-6.96053	0.068035	0.90445
34	6	-7.67987	-2.61422	0.658181
35	1	-5.64251	-2.94928	0.070864
36	6	-8.27281	-0.32986	1.163235
37	1	-6.68279	1.106121	1.029814
38	6	-8.63883	-1.6731	1.042307
39	1	-7.95448	-3.65576	0.553588
40	1	-9.00547	0.405925	1.46819
41	1	-9.65578	-1.98175	1.244417
42	1	3.020366	-2.7776	-2.23685
43	1	0.835344	5.865533	0.108708
44	6	3.987457	-1.04082	-0.43314
45	6	5.118969	-1.00616	0.005131
46	6	6.447896	-0.96313	0.520809
47	6	7.414277	-1.90196	0.101276
48	6	6.823493	0.019531	1.461413
49	6	8.711538	-1.85609	0.607811
50	1	7.134917	-2.6583	-0.61904
51	6	8.122903	0.058216	1.962996

52	1	6.089282	0.742766	1.788109
53	6	9.07153	-0.8776	1.539456
54	1	9.441426	-2.58284	0.276483
55	1	8.39581	0.817639	2.683724
56	1	10.07946	-0.84477	1.930848

TD-DFT analysis of 3p:



(a) (b)



(c) (d)

Figure S36: UV-VIS spectrum of **3p** in (a) MeCN, (b) $CHCl_3$, (c) MeOH and (d) DMSO calculated using Td-DFT.

Table S32: Some selected transitions in **3p** calculated from TD-DFT calculation.

Solvent	State	Transitions		Coefficient (%)	Energy (eV)	Wave Length (nm)	Oscillator strength
		From	To				
MeCN	S0→S1	HOMO	LUMO	69.61	3.2011	387.32	0.0261
	S0→S2	HOMO	LUMO+1	69.31	3.6526	339.44	0.8710
	S0→S3	HOMO	LUMO+2	67.33	3.9336	315.19	0.2819
	S0→S4	HOMO	LUMO+3	60.58	4.0558	305.69	0.3797

	S0→S5	HOMO–1	LUMO	59.43	4.1525	298.58	0.7057
$CHCL_3$	S0→S1	HOMO	LUMO	69.61	3.2011	387.32	0.0261
	S0→S2	HOMO	LUMO+1	69.31	3.6526	339.44	0.8710
	S0→S3	HOMO	LUMO+2	67.33	3.9336	315.19	0.2819
	S0→S4	HOMO	LUMO+3	60.58	4.0558	305.69	0.3797
	S0→S5	HOMO–1	LUMO	59.43	4.1525	298.58	0.7057
MeOH	S0→S1	HOMO	LUMO	69.61	3.1930	388.30	0.0240
	S0→S2	HOMO	LUMO+1	69.28	3.6636	338.42	0.8453
	S0→S3	HOMO	LUMO+2	67.70	3.9431	314.43	0.2531
	S0→S4	HOMO	LUMO+3	63.29	4.0654	304.98	0.3108
	S0→S5	HOMO–1	LUMO	61.97	4.1755	296.94	0.7741
DMSO	S0→S1	HOMO	LUMO	69.63	3.1909	388.56	0.0253
	S0→S2	HOMO	LUMO+1	69.30	3.6555	339.17	0.8650
	S0→S3	HOMO	LUMO+2	67.51	3.9374	314.89	0.2726
	S0→S4	HOMO	LUMO+3	61.91	4.0611	305.30	0.3430
	S0→S5	HOMO–1	LUMO	60.74	4.1624	297.86	0.7463

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