SUPPORTING INFORMATION

Phosphorescent cyclometalated platinum(II) complexes with phenyldiazine N^C ligands

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EXPERIMENTAL SECTION

General Methods

In air- and moisture-sensitive reactions, all glassware was flame-dried. All reactions were conducted under a dry nitrogen atmosphere using Schlenk techniques, but workups were used as received. The starting materials were purchased from Sigma-Aldrich, TCI or Alfa-Aesar and were used as received. ***Thin layer chromatography (TLC)*** was conducted on pre-coated aluminum sheets with 0.20 mm Merck Alugram SIL G/UV254 with fluorescent indicator UV254 and 0.25 mm Merck silica gel (60-F254). ***Column chromatography*** was carried out using *Sigma-Aldrich* silica gel 60 (particle size 63-200 μm) and Macherey Nagel Aluminum neutral oxide 40 (particle size 40-160 μm). ***Nuclear magnetic resonance (NMR) spectra*** were acquired at room temperature on a Bruker AC-300 spectrometer (^{1}H at 300 MHz, ^{13}C at 75 MHz,) and referenced as follows: ^{1}H NMR, residual $CHCl_3$ (δ = 7.26 ppm); $^{13}C\{^{1}H\}$ NMR, internal $CDCl_3$ (δ = 77.16 ppm). The chemical shifts δ are reported in parts per million relative to TMS (^{1}H, 0.0 ppm) and $CDCl_3$ (^{13}C, 77.16 ppm). The coupling constant *J* is given in Hz. In the ^{1}H NMR spectra, the following abbreviations are used to describe the peak pattern: *s* (singlet), *d* (doublet), *dd* (doublet of doublet), *t* (triplet), and *m* (multiplet). Acidic impurities in $CDCl_3$ were removed by treatment with anhydrous K_2CO_3. ***IR spectra*** were recorded on a Perkin-Elmer spectrum 100 spectrometer with an ATR sampling accessory. ***UV visible*** absorption spectra were recorded on a Jasco V-650 spectrophotometer. ***Emission spectra*** were measured on a Horiba Fluoromax spectrometer. Complexes were excited at their absorption maxima (band of lowest energy) to record the emission spectra in degassed DCM. The emission quantum yields of these complexes were calculated relative to 9,10 – Bis (phenylethynyl) anthracene in cyclohexane (Φ_{em} =1) as the reference solution.[1] The ***phosphorescence lifetimes*** measurements of deoxygenated DCM solutions samples were performed on the same spectrometer in the phosphorimeter mode. UV-vis and fluorescence spectra were recorded using standard 1 cm quartz cells. Stokes shifts were calculated by considering the lowest energetic absorption and the highest energy emission bands. ***High Resolution Mass Spectrometry (HRMS)*** analyses were performed at the "Centre Régional de Mesures Physiques de l'Ouest" (CRMPO, University of Rennes 1, France) using a Bruker MicroTOFQ II apparatus. ***Cyclic voltammetry*** The electrochemical studies were performed in a glovebox (Jacomex) (O_2 < 1 ppm, H_2O < 1 ppm) with a home-made 3-electrode cell (WE: Pt, RE: Ag wire, CE: Pt). Ferrocene was added at the end of each experiment to determine the redox potential values. The potential of the cell was controlled by an AUTOLAB PGSTAT 100 (Metrohm) potentiostat monitored by the NOVA© software (Metrohm). Dichloromethane was freshly distilled from CaH_2 and kept under Ar in the glovebox. The supporting salt NBu_4PF_6 Synthesized from NBu_4OH (Fluka) and HPF_6 (Aldrich). It was then purified, dried under vacuum for 48 hours at 100°C, and then kept under N_2 in the glovebox.

[1] M. Taniguchi and J. S. Lindsey, *Photochem. Photobiol.,* 2018, **94**, 290.

Computational Details.

DFT calculations were carried out using the Gaussian16 package,[2] employing the PBE0 functional,[3] together with the Def2-TZVP basis set with a relativistic pseudopotential for Pt, from EMSL Basis Set Exchange Library.[4] Implicit solvent (chloroform) effects were included in all calculations through the polarizable continuum model (PCM).[5] The optimized geometries were fully characterized as true minima by analytical frequency calculations (no imaginary values). The geometries obtained from DFT calculations were used to perform natural atomic charge analysis with the NBO 6.0 program.[6] The ionization energies and electron affinities were computed as the difference between the energies of the corresponding cation and anion, respectively, and that of the neutral complex. These energies were taken after full geometry optimizations, on the minima of these three potential-energy surfaces and with equilibrium solvation. TD-DFT calculations were carried out at the same level of calculations. The graphical SWizard program[7] was used for simulating UV-vis spectra. TD-DFT calculations found the lowest triplet state to result from a HOMO-LUMO transition. Thus, phosphorescence was assumed to occur from this triplet state, which was fully optimized at the PBE0/Def2-TZVP level. The phosphorescence emission spectra were computed within the Franck-Condon principle by using the Adiabatic Hessian method[8] which takes into account vibrational mode mixing and a proper description of both optimized ground and excited (triplet) states potential energy surfaces. The lowest normal modes in the vibronic treatment were neglected in order to obtain sufficient spectrum progression. We employed the class-based pre-screening to limit the number of terms involved in the vibronic calculation with the following settings: Cmax1 = 70,

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[2] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[3] a) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865–3868; b) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1997, **78**, 1396–1396; d) C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158–6170.

[4] a) A. Schäfer, H. Horn and R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571–2577; b) A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829–5835.

[5] a) J. Tomasi, R. Cammi, B. Mennucci, C. Cappelli and S. Corni, *Phys. Chem. Chem. Phys.*, 2002, **4**, 5697–5712; b) J. Tomasi, B. Mennucci and R. Cammi, *Chem Rev*, 2005, **105**, 2999–3093.

[6] E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, F. Weinhold, NBO 6.0; Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2013, http://nbo6.chem.wisc.edu.

[7] a) S. I. Gorelsky, SWizard program, http://www.sg-chem.net/, University of Ottawa, Ottawa, Canada, 2013; b) S. I. Gorelsky and A. B. P. Lever, *J. Organomet. Chem.*, 2001, **635**, 187–196.

[8] a) M. Cossi, V. Barone, R. Cammi and J. Tomasi, *Chem. Phys. Lett.*, 1996, **255**, 327–335; b) V. Barone, M. Cossi and J. Tomasi, *J. Chem. Phys.*, 1997, **107**, 3210–3221.

Cmax2 = 70, Nmax1 = 100 × 108.[9] All the vibronic plots were realized using the VMS piece of software.[10] Charge transfers associated with the triplet→singlet emissive transitions were illustrated by plots of the differences between the densities of the excited and ground states and quantified by associated charge transfer values and distances as defined by Adamo and co-workers.[11]

X-ray Structure Determination

The SCXRD studies of **7** (CCDC 2211426), **12** (CCDC 2211427) and **14** (CCDC 2211428) were performed on an APEXII, Bruker AXS diffractometer equipped with a CCD plate detector and a Mo-Kα radiation (λ = 0.71073 Å, graphite monochromator). Measurements were done at 150K. Crystal structures were solved by dual-space algorithm using the SHELXT program,[12] and then refined with full-matrix least-square methods based on F^2 (SHELXL).[13] All non hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in the structural model in their calculated positions, and constrained to ride on the attached carbon atom. Relevant collection and refinement data for all compounds are given in the Supporting Information. All data can be obtained from the Cambridge Structural Database via www.ccdc.cam.ac.uk/data_request/cif.

[9] a) F. Santoro, R. Improta, A. Lami, J. Bloino and V. Barone, *J. Chem. Phys.*, 2007, **126**, 084509; b) F. Santoro, A. Lami, R. Improta and V. Barone, *J. Chem. Phys.*, 2007, **126**, 184102; c) F. Santoro, A. Lami, R. Improta, J. Bloino and V. Barone, *J. Chem. Phys.*, 2008, **128**, 224311.

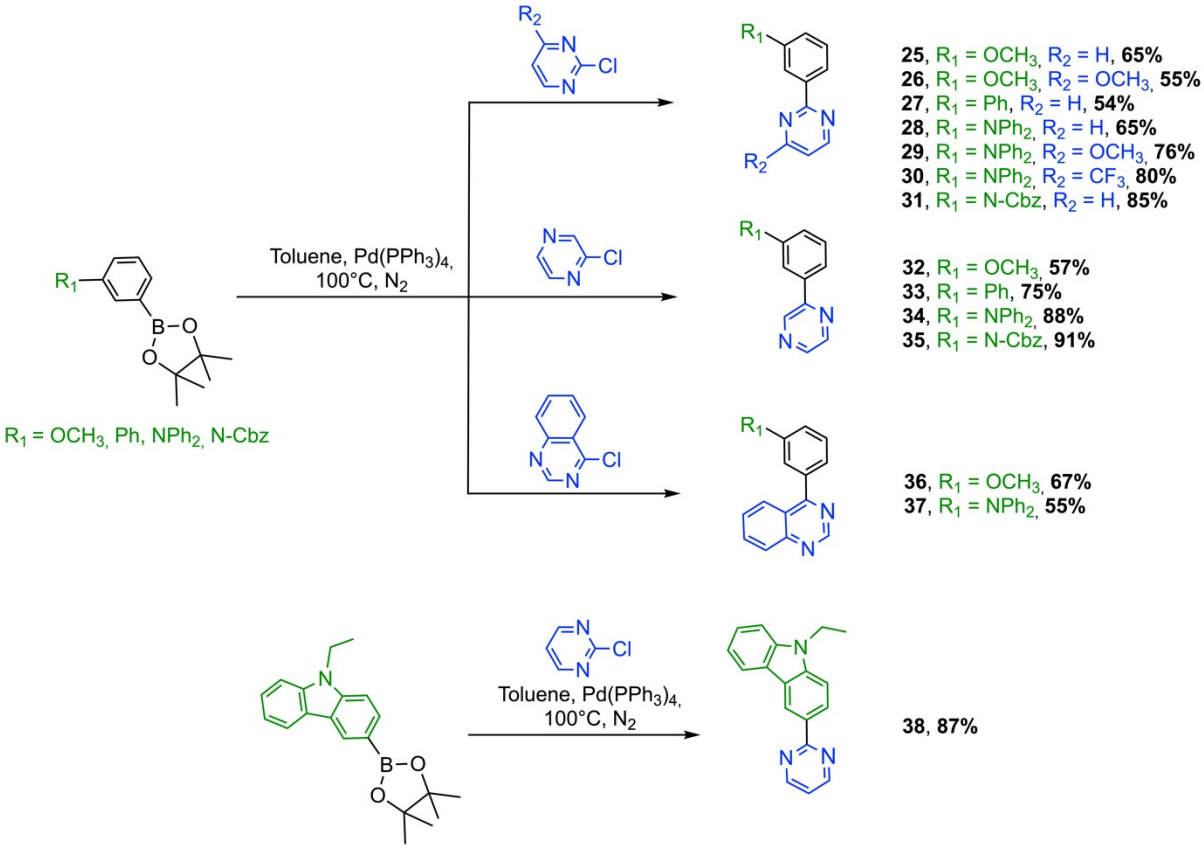
[10] Licari, A. Baiardi, M. Biczysko, F. Egidi, C. Latouche and V. Barone, *J. Comput. Chem.*, 2015, **36**, 321–334.

[11] a) T. Le Bahers, C. Adamo and I. Ciofini, *J. Chem. Theory Comput.*, **2011**, *7*, 2498–2506; b) I. Ciofini, T. Le Bahers, C. Adamo, F. Odobel and D. Jacquemin, *J. Phys. Chem. C*, 2012, **116**, 11946–11955; c) D. Jacquemin, T. Le Bahers, C. Adamo and I. Ciofini, *Phys. Chem. Chem. Phys.*, 2012, **14**, 5383–5388.

[12] G. M. Sheldrick, SHELXT - Integrated Space-group and Crystal-structure Determination. *Acta Cryst.,* 2015, **A71**, 3.

[13] G. M. Sheldrick, Crystal Structure Refinement with SHELXL. Acta Cryst. 2015, **C71**, 3.

Synthesis of Ligands 25-38



Scheme S1: Synthesis of ligands **25-38**.

***General procedure Suzuki cross coupling reaction*:** Chlorodiazine derivatives (1.1 equiv) and corresponding pinacol ester (1 equiv) were dissolved in toluene (20mL), and nitrogen was bubbled through the solution for 10 min. $Pd(PPh_3)_4$ (5 %) and 20% aqueous K_2CO_3 were added, and then the reaction was reflux for 15h. The reaction mixture was cooled to room temperature and diluted with EtOAc/aqueous NH_4Cl (1:1, 100 mL). Organic layer was separated, and the aqueous one was extracted with EtOAc (2 × 50 mL). The combined organic extracts were dried over anhydrous $MgSO_4$ and solvent was evaporated under reduced pressure. The solid residue was purified by silica gel column chromatography (indicated solvents).

***2-(3-methoxyphenyl)pyrimidine* (25):** Synthesized from 2-chloropyrimidine (252 mg, 2.2 mmol) and 3-methoxyphenylboronic acid pinacol ester (470 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 9:1, v/v) to give compound **25** as a pale yellow oil that slowly crystallizes in 65% yield (243 mg). Spectroscopic data were similar to literature.[14]

[14] M. Fecková, S. Kahlal, T. Roisnel, J.-Y. Saillard, J. Boixel, M. Hruzd, P. le Poul, S. Gauthier, F. Robin-le Guen, F. Bureš, S. Achelle, *Eur. J. Inorg. Chem.* 2021, 1592.

***4-methoxy-2-(3-methoxyphenyl)pyrimidine* (26):** Synthesized from 2-chloro-4-methoxypyrimidine (318 mg, 2.2 mmol) and 3-methoxyphenylboronic acid pinacol ester (470 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 9:1, v/v) to give compound **26** as a pale-yellow oil in 55% yield (240 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 8.45 (d, $^3J_{HH}$ = 5.7 Hz, 1H), 8.09–8.03 (m, 1H), 8.03–7.99 (m, 1H), 7.37 (t, $^3J_{HH}$ = 7.9 Hz, 1H), 7.01 (dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.6 Hz, 1H), 6.57 (d, $^3J_{HH}$ = 5.7 Hz, 1H), 4.02 (s, 3H), 3.86 (s, 3H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 168.9 (C), 163.6 (C), 159.4 (C), 156.8 (CH), 138.5 (C), 128.9 (CH), 120.3 (CH), 116.4 (CH), 112.6(CH), 105.8 (CH), 54.8 (OCH_3), 52.9 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{12}H_{13}N_2O_2$ $[M+Na]^+$: 217.0972, found: 217.0974 (1 ppm).

***2-([1,1'-biphenyl]-3-yl)pyrimidine* (27):** Synthesized from 2-chloropyrimidine (252 mg, 2.2 mmol) and 3-biphenylboronic acid pinacol ester (561 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 8:2, v/v) to give compound **27** as white solid in 54% yield (251 mg). CAS Number: 377047-38-6. NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 8.61 – 8.46 (m, 3H), 8.27 (dt, $^3J_{HH}$ = 7.9 Hz, $^3J_{HH}$ = 1.4 Hz, 1H), 7.54 – 7.41 (m, 3H), 7.35 – 7.27 (m, 1H), 7.25 – 7.17 (m, 2H), 7.16 – 7.07 (m, 1H), 6.91 (t, $^3J_{HH}$ = 4.8 Hz, 1H).

***N,N-diphenyl-3-(pyrimidin-2-yl)aniline* (28) :** Synthesized from 2-chloropyrimidine (252 mg, 2.2 mmol) and 4-(Diphenylamino)phenylboronic acid pinacol ester (743 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 9:1, v/v) to give compound **28** as pale-yellow solid in 65% yield (421 mg). Spectroscopic data were similar to literature.[12]

***3-(4-methoxypyrimidin-2-yl)-N,N-diphenylaniline* (29):** Synthesized from 2-chloro-4-methoxypyrimidine (318 mg, 2.2 mmol) and 4-(Diphenylamino)phenylboronic acid pinacol ester (743 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (DCM) to give compound **29** as pale-yellow solid in 76% yield (538 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 8.47 (d, $^3J_{HH}$ = 5.7 Hz, 1H), 8.43 – 8.37 (m, 1H), 8.29 – 8.20 (m, 1H), 7.45 (t, $^3J_{HH}$ = 7.9 Hz, 1H), 7.39 – 7.23 (m, 9H), 7.14 – 7.05 (m, 2H), 6.61 (d, $^3J_{HH}$ = 5.7 Hz, 1H), 4.02 (s, 3H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 168.9 (C), 163.7 (C), 156.8 (CH), 147.7 (C), 147.4 (C), 138.5 (C), 128.9 (CH), 128.8 (CH), 126.1 (CH), 123.8 (CH), 123.4 (CH), 122.4 (CH), 122.2 (CH), 105.7 (CH), 52.9 (CH_3); HRMS (ESI) *m/z* calculated for $C_{23}H_{20}N_3O$ $[M+H]^+$: 354.1609, found: 354.1606 (1 ppm).

***N,N-diphenyl-3-(4-(trifluoromethyl)pyrimidin-2-yl)aniline* (30):** Synthesized from 2-chloro-4-(trifluoromethyl)pyrimidine (402 mg, 2.2 mmol) and 4-(diphenylamino)phenylboronic acid pinacol ester (743 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 10:1, v/v) to give compound **30** as pale-yellow solid in 80% yield (627 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz) : 8.96 (d, $^3J_{HH}$ = 5.0 Hz, 1H), 8.37 (t, $^4J_{HH}$ = 2.0 Hz, 1H), 8.25 (dt, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.2 Hz, 1H), 7.51–7.46 (m, 1H), 7.46–7.41 (m, 1H), 7.38–7.29 (m, 5H), 7.26–7.18 (m, 4H), 7.14–7.06 (m, 2H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 164.9 (C), 159.1 (CH), 155.9 (C, q, $^2J_{CF}$ = 36.2 Hz), 148.2 (C), 147.4 (C), 137.2 (C), 129.4 (CH), 129.0 (CH), 128.9 (CH), 127.1 (CH), 123.9 (CH), 123.7 (CH), 123.4 (CH), 122.7 (CH), 120.6 (CF_3, q, $^1J_{CF}$ = 273 Hz), 114.0 (CH); HRMS (ESI) *m/z* calculated for $C_{23}H_{17}N_3F_3$ $[M+H]^+$: 392.1369, found: 392.1364 (1 ppm).

9-(3-(pyrimidin-2-yl)phenyl)-9H-carbazole **(31):** Synthesized from 2-chloropyrimidine (252 mg, 2.2 mmol) and 9-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9H-carbazole (740 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 8:2, v/v) to give compound **31** as white solid in 85% yield (547 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 8.85 – 8.71 (m, 3H), 8.60 (dt, $^3J_{HH}$ = 7.0 Hz, $^4J_{HH}$ = 1.8 Hz, 1H), 8.25 – 8.16 (m, 1H), 7.81 – 7.67 (m, 2H), 7.57 – 7.42 (m, 4H), 7.34 (td, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.3 Hz, 2H), 7.18 (t, $^3J_{HH}$ = 4.8 Hz, 1H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 163.6 (C), 157.0 (CH), 140.6 (C), 139.4 (C), 138.8 (C), 129.8 (CH), 129.0 (CH), 126.8 (CH), 125.7 (CH), 123.1 (C), 120.0 (CH), 119.7 (CH), 119.1 (CH), 109.6 (CH). HRMS (ESI) *m/z* calculated for $C_{22}H_{16}N_3$ $[M+H]^+$: 322.1339, found: 322.1341 (1 ppm).

2-(3-methoxyphenyl)pyrazine **(32):** Synthesized from 2-chloropyrazine (252 mg, 0.2 ml, 2.2 mmol) and 3-methoxyphenylboronic acid pinacol ester (470 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 10:1, v/v) to give compound **32** as a pale yellow oil in 57% yield (215 mg). Spectroscopic data were similar to literature.[15]

2-([1,1'-biphenyl]-3-yl)pyrazine **(33):** Synthesized from 2-chloropyrazine (252 mg, 2.2 mmol) and 3-biphenylboronic acid pinacol ester (561 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 8:2, v/v) to give compound **33** as white solid in 75% yield (350 mg). CAS Number: 2366147-92-2. NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.06 (d, $^4J_{HH}$ = 1.6 Hz, 1H), 8.58 (dd, $^3J_{HH}$ = 2.5 Hz, $^4J_{HH}$ =1.6 Hz, 1H), 8.46 (d, $^3J_{HH}$ = 2.5 Hz, 1H), 8.27 (t, $^4J_{HH}$ = 1.8 Hz, 1H), 7.95 (dt, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 1.5 Hz, 1H), 7.70 – 7.61 (m, 3H), 7.52 (d, $^3J_{HH}$ = 7.8 Hz, 1H), 7.49 – 7.40 (m, 2H), 7.40 – 7.32 (m, 1H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 151.7(C), 143.4(CH), 142.3(CH), 141.5(CH), 141.2(C), 139.8(C), 136.1(C), 128.7(CH), 128.2(CH), 127.8(CH), 126.9(CH), 126.5(CH), 125.0(CH), 125.0(CH).

N,N-diphenyl-3-(pyrazin-2-yl)aniline **(34):** Synthesized from 2-chloropyrazine (252 mg, 0.2 ml, 2.2 mmol) and 4-(Diphenylamino)phenylboronic acid pinacol ester (743 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 9:1, v/v) to give compound **34** as pale yellow solid in 88% yield (570 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 8.92 (s, 1H), 8.57 (d, $^3J_{HH}$ = 2.6 Hz, 1H), 8.47 (d, $^3J_{HH}$ = 2.6 Hz, 1H), 7.80–7.75 (m, 1H), 7.67–7.60 (m, 1H), 7.38 (t, $^3J_{HH}$ = 7.9 Hz, 1H), 7.32–7.25 (m, 4H), 7.23–7.12 (m, 5H), 7.06 (tt, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.2 Hz 2H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 152.2 (C), 148.4 (C), 147.2 (C), 143.7 (CH), 142.5 (CH), 141.9(CH), 137.2 (C), 129.5 (CH), 129.0 (CH), 124.8 (CH), 124.1 (CH), 122.8 (CH), 121.7 (CH), 120.6 (CH); HRMS (ESI) *m/z* calculated for $C_{22}H_{18}N_3$ $[M+H]^+$: 324.1495, found: 324.1497 (1 ppm).

9-(3-(pyrazin-2-yl)phenyl)-9H-carbazole **(35):** Synthesized from 2-chloropyrazine (252 mg, 2.2 mmol) and 9-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9H-carbazole (740 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 8:2, v/v) to give compound **35** as white solid in 91% yield (585 mg).NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.09 (s, 1H), 8.64 (s, 1H), 8.56 (s, 1H), 8.30 (s, 1H), 8.24–8.09 (m, 3H), 7.79–7.65 (m, 2H),

[15] S. Yanagisawa, K. Ueda, T. Taniguchi and K. Itami, *Org. Lett.*, 2008, **10**, 4673.

7.52–7.40 (m, 4H), 7.38–7.30 (m, 2H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$):151.5 (C), 144.0 (CH), 143.1 (CH), 141.9 (CH), 140.1 (C), 138.2 (C), 138.0 (C), 130.2 (CH), 128.1 (CH), 125.8 (CH), 125.4 (CH), 125.3 (CH), 123.2 (C), 120.1 (CH), 119.8 (CH), 109.4 (CH); HRMS (ESI) *m/z* calculated for $C_{22}H_{16}N_3$ $[M+H]^+$: 322.1338, found: 322.1338 (0 ppm).

4-(3-methoxyphenyl)quinazoline **(36):** Synthesized from 4-chloroquinazoline (363 mg, 2.2 mmol) and 3-methoxyphenylboronic acid pinacol ester (470 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 8:2, v/v) to give compound **36** as a pale-yellow oil in 67% yield (317 mg). Spectroscopic data were similar to literature.[16]

N,N-diphenyl-3-(quinazolin-4-yl)aniline **(37):** Synthesized from 4-chloroquinazoline (363 mg, 2.2 mmol) and 4-(diphenylamino)phenylboronic acid pinacol ester (743 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 9:1, v/v) to give compound **37** as pale yellow solid in 55% yield (411 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.33 (s, 1H), 8.07 (d, $^3J_{HH}$ = 8.5 Hz, 2H), 7.86 (td, $^3J_{HH}$ = 6.9 Hz, $^4J_{HH}$ = 1.2, 1H), 7.55 (td, $^3J_{HH}$ = 6.9 Hz, $^4J_{HH}$ = 1.2, 1H), 7.48–7.36 (m, 3H), 7.33–7.23 (m, 5H), 7.22–7.15 (m, 4H), 7.08–6.98 (m, 2H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 167.6 (C), 154.3 (CH), 150.7 (C), 142.2 (C), 147.1 (C), 137.8 (C), 133.3 (CH), 129.3 (CH), 129.1 (CH), 128.5 (CH), 127.2 (CH), 126.7 (CH), 124.5 (CH), 124.4 (CH), 124.3 (CH), 123.4 (CH), 123.0 (CH), 122.4(C); HRMS (ESI) *m/z* calculated for $C_{26}H_{20}N_3$ $[M+H]^+$: 374.1652, found: 374.1654 (1 ppm).

9-ethyl-2-(pyrimidin-2-yl)-9H-carbazole **(38)** Synthesized from 2-chloropyrimidine (252 mg, 2.2 mmol) and 9-Ethyl-*9H*-carbazol-3-boronic acid pinacol ester (643 mg, 2 mmol) following the general procedure Suzuki cross coupling. The crude product was purified by silica gel column chromatography (Petroleum ether /EtOAc, 7:3, v/v) to give compound **38** as a white solid in 87% yield (476 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 8.85 (d, $^3J_{HH}$ = 4.8 Hz, 2H), 8.57 (s, 1H), 8.39 (d, $^3J_{HH}$ = 8.2 Hz, 1H), 8.27–8.11 (m, 2H), 7.56–7.39 (m, 2H), 7.26 (t, $^3J_{HH}$ = 7.2 Hz, 1H), 7.18 (t, $^3J_{HH}$ = 4.8 Hz, 1H), 4.49 (q, $^3J_{HH}$ = 7.2 Hz, 2H), 1.50 (t, $^3J_{HH}$ = 7.2 Hz, 3H). $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 166.1 (C), 157.8 (CH), 141.6 (C), 140.3 (C), 135.6 (C), 126.9 (CH), 125.8 (C), 124.0 (CH), 121.5 (C), 120.9 (CH), 119.7 (CH), 119.6 (CH), 119.3 (CH), 109.2 (CH), 109.0 (CH), 38.2 (CH_2), 14.6 (CH_3). HRMS (ESI) *m/z* calculated for $C_{18}H_{16}N_3$ $[M+H]^+$: 274.1339, found: 274.1340 (0 ppm).

Synthesis of Complexes 1-24

[16] S. S. Yan, B. Yu and H.-M. Liu, *Chem.-Eur. J.,* 2009, **25**, 13109.

***General procedure for the synthesis of Pt^{II} complexes*:** K_2PtCl_4 (1 equiv) and ligand (1.2 equiv) were dissolved in a mixture of 2-ethoxyethanol/H_2O (3:1, 20 mL). The mixture was bubbled with nitrogen for 10 min and then stirred at 90 °C for 15h. The solution was cooled to room temperature and diluted with H_2O, precipitate was filtrated off, and dried under vacuum. μ-Chloro-bridged intermediate was dissolved in $CHCl_3$ and pyridine (or 4-methoxypyridine / pyrimidine) was added (2.5 equiv). The mixture was stirred at 50 °C for 15h. The reaction mixture was cooled to room temperature and diluted with CH_2Cl_2/aqueous NH_4Cl (1:1, 100 mL). Organic layer was separated, and the aqueous one was extracted with CH_2Cl_2 (2 × 50 mL). The combined organic extracts were dried over anhydrous $MgSO_4$ and solvent was evaporated under reduced pressure. The solid residue was purified by silica gel column chromatography (EtOAc/CH_2Cl_2, from 1:10 to 1:1, v/v).

***Complex 1*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **25** (54 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **1** was obtained as a yellow powder. Yield : 44 % (53 mg). Spectroscopic data were similar to literature.[12]

***Complex 2*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **25** (54 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **2** was obtained as a orange-yellow powder in yield 38 % (48 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.75 (dd, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 2.2 Hz, $^3J_{PtH}$ = 57 Hz, 1H), 8.75 (m, $^3J_{PtH}$ = 46.4 Hz, 3H), 7.40 (d, $^4J_{HH}$ = 2.9 Hz, 1H), 7.05 (t, $^3J_{HH}$ = 5.9 Hz, 1H), 6.97–6.86 (m, 2H), 6.73 (dd, $^3J_{HH}$ = 8.4Hz , $^4J_{HH}$ = 2.9 Hz, 1H), 6.34 (d, $^3J_{HH}$ = 8.4 Hz, $^3J_{PtH}$ = 47.1 Hz, 1H), 3.93 (s, 3H), 3.82 (s, 3H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 175.3 (C), 166.1 (C), 157.8 (CH), 157.2 (CH), 156.6 (C), 154.2 (CH), 141.7 (C), 131.6 (C), 130.8 (CH; $^2J_{PtC}$ = 59.2 Hz), 119.7 (CH), 117.2 (CH), 111.8 (CH; $^2J_{PtC}$ = 54.2 Hz), 110.9 (CH), 55.6 (OCH_3), 55.1 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{17}H_{16}N_3O_2{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 547.0471, found: 547.0468 (1 ppm).

***Complex 3*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **25** (63 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **3** was obtained as a yellow powder. Yield : 43 % (55 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.30 (d, $^3J_{HH}$ = 6.7 Hz, $^3J_{PtH}$ = 32.7 Hz, 1H), 9.02 (d, $^3J_{HH}$ = 3.5 Hz, $^3J_{PtH}$ = 42 Hz, 2H), 7.86 (t, $^3J_{HH}$ = 7.7 Hz, 1H), 7.53–7.30 (m, 3H), 6.69 (dd, $^3J_{HH}$ = 8.3, $^4J_{HH}$ = 2.9 Hz, 1H), 6.49 (d, $^3J_{HH}$ = 6.7 Hz, 1H), 6.24 (d, $^3J_{HH}$ = 8.4 Hz, $^3J_{PtH}$ = 39.6 Hz, 1H), 4.10 (s, 3H), 3.79 (s, 3H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 175.4 (C), 169.6 (C), 156.3 (CH), 156.2 (C), 153.8 (CH), 142.1 (C), 137.3 (CH), 131.3 (C), 130.3 (CH; $^2J_{PtC}$ = 58.8 Hz), 125.6 (CH; $^3J_{PtC}$ = 47.2 Hz), 118.4 (CH; $^2J_{PtC}$ = 60 Hz), 111.7 (CH; $^2J_{PtC}$ = 52 Hz), 104.2 (CH), 55.0 (OCH_3), 54.1 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{17}H_{16}N_3O_2{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 547.0471, found: 547.0464 (1 ppm).

***Complex 4*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **26** (63 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for

the synthesis of Pt^{II} complexes. The complex **4** was obtained as a yellow powder. Yield: 27 % (36 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.35 (d, $^3J_{HH}$ = 6.7 Hz, $^3J_{PtH}$ = 38.4 Hz, 1H), 8.78 (d, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.5 Hz, $^3J_{PtH}$ = 41.1 Hz, 2H), 7.39 (d, $^4J_{HH}$ = 2.9 Hz, 1H), 6.90 (d, $^3J_{HH}$ = 7.2 Hz, 2H), 6.73 (dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.9 Hz, 1H), 6.52 (d, $^3J_{HH}$ = 6.7 Hz, 1H), 6.36 (d, $^3J_{HH}$ = 8.4 Hz, $^3J_{PtH}$ = 48 Hz, 1H), 4.12 (s, 3H), 3.94 (s, 3H), 3.81 (s, 3H).$^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 170.4 (C), 166.8 (C), 157.4 (CH), 157.2 (C), 155.2 (CH), 132.3 (C), 131.5 (CH), 126.1 (CH), 119.5 (CH), 112.5 (CH; $^2J_{PtC}$ = 54 Hz), 105.1(CH), 56.6(OCH_3), 56.0(OCH_3), 55.0(OCH_3); HRMS (ESI) *m/z* calculated for $C_{18}H_{18}N_3O_3{}^{195}Pt$ [M -.Cl]$^+$: 519.0991, found: 519.0997 (1 ppm).

***Complex 5*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **26** (63 mg, 0.29 mmol) and pyrimidine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **5** was obtained as a light green-yellow powder. Yield: 27 % (35 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.67 (s, $^3J_{PtH}$ = 26.4 Hz, 1H), 9.29 (d, $^3J_{HH}$ = 6.7 Hz, 2H), 8.90 (dd, $^3J_{HH}$ = 4.9 Hz, $^4J_{HH}$ = 2.2 Hz, $^3J_{PtH}$ = 43.8 Hz, 1H), 7.56–7.43 (m, 1H), 7.38 (d, $^4J_{HH}$ = 2.9 Hz, 1H), 6.74 (dd, $^3J_{HH}$ = 8.3 Hz, $^4J_{HH}$ = 2.9 Hz, 1H), 6.53 (d, $^3J_{HH}$ = 6.7 Hz, 1H), 6.28 (d, $^3J_{HH}$ = 8.3 Hz, 1H), 4.12 (s, 3H), 3.81 (s, 3H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 169.6 (C), 160.5 (CH), 157.1 (CH), 156.5 (C), 156.3 (CH), 142.2 (C), 130.0 (CH), 122.1 (CH), 118.5 (CH), 112.1 (CH), 104.5 (CH), 55.09 (OCH_3), 54.21 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{16}H_{15}N_4O_2{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 548.0424, found: 548.0429 (1 ppm).

***Complex 6*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **28** (94 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **6** was obtained as a orange powder in yield 77 % (117 mg). Spectroscopic data were similar to literature.[12]

***Complex 7*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **29** (94 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **7** was obtained as a orange powder. Yield: 56% (90 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.78 (dd, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 2.2 Hz, $^3J_{PtH}$ = 32.4 Hz, 1H), 8.75 (d, $^3J_{HH}$ = 7.2 Hz, 2H), 8.66 (dd, $^3J_{HH}$ = 4.8 Hz, $^4J_{HH}$ = 2.2 Hz, 1H), 7.67 (d, $^4J_{HH}$ = 2.6 Hz, 1H), 7.27 – 7.15 (m, 4H), 7.06-7.04 (m, 5H), 6.96-6.89 (m, 5H), 6.39 (d, $^3J_{HH}$ = 8.2 Hz, $^3J_{PtH}$ = 47.6 Hz, 1H), 3.91 (s, 3H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 175.0 (C), 166.1 (C), 157.8 (CH), 157.2 (CH), 154.1 (CH), 147.4 (C), 142.2 (C), 144.0 (C), 135.0 (C), 131.0 (CH), 129.3 (CH), 128.8 (CH), 124.0 (CH), 123.0 (CH), 121.9 (CH), 117.3 (CH), 111.1 (CH; $^2J_{PtC}$ = 54.3 Hz), 55.7 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{28}H_{23}N_4O^{35}ClNa^{195}Pt$ $[M+Na]^+$: 684.1100, found: 684.1092 (1 ppm).

***Complex 8*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **28** (103 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **8** was obtained as a orange powder. Yield: 62 % (100

mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.37 (d, $^3J_{HH}$ = 6.7 Hz, $^3J_{PtH}$ = 33.3 Hz, 1H), 9.00 (dd, $^3J_{HH}$ = 6.5 Hz, $^4J_{HH}$ = 1.5 Hz, $^3J_{PtH}$ = 41.7 Hz, 2H), 7.87 (tt, $^3J_{HH}$ = 7.9 Hz, $^4J_{HH}$ = 1.5 Hz, 1H), 7.63 (d, $^4J_{HH}$ = 2.6 Hz, 1H), 7.45–7.34 (m, 2H), 7.21–7.16 (m, 4H), 7.11–7.01 (m, 4H), 6.9 –6.91 (m, 2H), 6.86 (dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.6 Hz, 1H), 6.53 (d, $^3J_{HH}$ = 6.7 Hz, 1H), 6.31 (d, $^3J_{HH}$ = 8.2 Hz, $^3J_{PtH}$ = 46.5 Hz, 1H), 3.97 (s, 3H). ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 170.4 (C), 157.4 (CH), 154.7 (CH), 148.3 (C), 144.4 (C), 143.5 (C), 138.3 (CH), 136.3 (C), 131.6 (CH), 130.7 (CH), 129.7 (CH), 126.5 (CH), 125.2 (CH), 124.7 (C), 123.7 (CH), 122.6 (CH), 105.3 (CH), 55.1 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{28}H_{23}N_4O^{35}ClNa^{195}Pt$ $[M+Na]^+$: 684.1100, found: 684.1098 (0 ppm).

***Complex 9*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **29** (103 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **9** was obtained as a orange powder. Yield: 66% (110 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.37 (d, $^3J_{HH}$ = 6.7 Hz, $^3J_{PtH}$ = 26.7 Hz, 1H), 8.77 (dd, $^3J_{HH}$ = 7.1 Hz, $^4J_{HH}$ = 1.5 Hz, $^3J_{PtH}$ = 38.7 Hz, 2H), 7.62 (d, $^4J_{HH}$ = 2.6 Hz, 1H), 7.24 – 7.15 (m, 4H), 7.09–7.02 (m, 4H), 6.99–6.83 (m, 5H), 6.52 (d, $^3J_{HH}$ = 6.7 Hz, 1H), 6.40 (d, $^3J_{HH}$ = 7.1 Hz, 1H), 3.97 (s, 3H), 3.92 (s, 3H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 175.3 (C), 169.5 (C), 166.0 (C), 156.5 (CH), 154.3 (CH), 147.4 (C), 143.3 (C), 142.7 (C), 135.5 (C), 131.0 (CH), 129.9 (CH), 128.8 (CH), 124.3 (CH), 122.8 (CH), 121.7 (CH), 111.3 (CH), 104.4 (CH), 55.7 (OCH_3), 54.2 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{29}H_{25}N_4O_2{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 714.1206, found: 714.1202 (1 ppm).

***Complex 10*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **29** (103 mg, 0.29 mmol) and pyrimidine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **10** was obtained as a yellow-orange powder. Yield: 54 % (86 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.69 (s, $^3J_{PtH}$ = 24.9 Hz, 1H), 9.4 –9.17 (m, 2H), 8.89 (dd, $^3J_{HH}$ = 4.9 Hz, $^4J_{HH}$ = 2.2 Hz, 1H), 7.63 (d, $^4J_{HH}$ = 2.5Hz, 1H), 7.54–7.39 (m, 1H), 7.28–7.16 (m, 4H), 7.13–7.04 (m, 4H), 7.00–6.86 (m, 3H), 6.54 (d, $^3J_{HH}$ = 6.8 Hz, 1H), 6.33 (d, $^3J_{HH}$ = 8.2 Hz, $^3J_{PtH}$ = 45.6 Hz, 1H), 3.98 (s, 3H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 169.5 (C), 160.3 (CH), 157.2 (CH), 156.4 (CH), 147.3 (C), 143.9 (C), 142.4 (C), 134.5 (C), 130.6 (CH), 130.3 (CH), 129.6 (CH), 128.8 (CH), 124.2 (CH), 122.9 (CH), 122.1 (CH), 121.9 (CH), 104.6 (CH), 54.3 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{27}H_{22}N_5O^{35}Cl^{195}Pt$ $[M^{+\bullet}]$: 662.1156, found: 662.1158 (0 ppm).

***Complex 11*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **30** (114 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **11** was obtained as a orange powder. Yield: 55 % (93 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 10.09 (d, $^3J_{HH}$ = 6.0 Hz, $^3J_{PtH}$ = 39.6 Hz, 1H), 8.94 (d, $^3J_{HH}$ = 4.9 Hz, $^3J_{PtH}$ = 44.7 Hz, 2H), 7.89 (tt, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ =1.6 Hz, 1H), 7.74 (d, $^3J_{HH}$ = 2.6 Hz, $^4J_{PtH}$ = 40.2 Hz, 1H), 7.48–7.40 (m, 2H), 7.34 (d, $^3J_{HH}$ = 5.9 Hz, 1H), 7.25–7.13 (m, 4H), 7.07–6.99 (m, 4H), 6.99–6.89 (m, 3H), 6.31 (d, $^3J_{HH}$ = 8.2 Hz, $^3J_{PtH}$ = 39.9 Hz, 1H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 159.7 (CH), 153.7 (CH), 147.3 (C), 144.3 (C), 140.7 (C), 138.3 (C), 138.0 (CH), 136.3 (C), 131.1 (CH), 130.8 (CH), 128.9 (CH), 125.9 (CH), 125.0 (CH), 123.0 (CH), 122.1 (CH), 121.7 (C), 113.2 (CH); HRMS (ESI) *m/z* calculated for $C_{28}H_{20}N_4F_3{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 722.0869, found: 722.0862 (1 ppm).

***Complex 12*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **27** (68 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the

synthesis of Pt^{II} complexes. The complex **12** was obtained as a yellow powder. Yield: 66 % (87 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.80 (dd, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 2.2 Hz, $^3J_{PtH}$ = 21 Hz, 1H), 9.04 (d, $^3J_{HH}$ = 5.0 Hz, $^3J_{PtH}$ = 25.2 Hz, 2H), 8.77 (dd, $^3J_{HH}$ = 4.8 Hz, $^4J_{HH}$ = 2.3 Hz, 1H), 8.11 (d, $^4J_{HH}$ = 2.2 Hz, 1H), 7.92 (tt, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 1.6 Hz, 1H), 7.67–7.59 (m, 2H), 7.50–7.39 (m, 4H), 7.38–7.29 (m, 2H), 7.09 (dd, $^3J_{HH}$ = 5.9, $^3J_{HH}$ = 4.7 Hz, 1H), 6.46 (d, $^3J_{HH}$ = 8.0 Hz, $^3J_{PtH}$ = 47.7 Hz, 1H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 158.0 (CH), 157.2 (CH), 153.8 (CH), 141.7 (C), 140.4 (C), 139.8 (C), 137.7 (CH), 136.5 (C), 131.7 (C), 130.5 (CH), 130.4 (CH), 129.0 (CH), 126.7 (CH), 126.3 (CH), 126.1 (CH), 125.8 (CH), 125.7 (CH), 117.4 (CH); HRMS (ESI) *m/z* calculated for $C_{21}H_{16}N_3{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 563.0573, found: 563.0569 (1 ppm).

***Complex 13*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **27** (68 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **13** was obtained as a yellow powder. Yield: 65% (85 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.67 (dd, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 2.2 Hz, $^3J_{PtH}$ = 34 Hz, 1H), 8.82 (d, $^3J_{HH}$ = 5.2 Hz, $^3J_{PtH}$ = 40.2 Hz, 2H), 8.64 (dd, $^3J_{HH}$ = 4.7 Hz, $^4J_{HH}$ = 2.2 Hz, 1H), 8.03 (s, 1H), 7.68–7.57 (m, 2H), 7.46–7.36 (m, 2H), 7.35–7.27 (m, 2H), 7.00–6.92 (m, 1H), 6.92–6.86 (m, 2H), 6.48 (d, $^3J_{HH}$ = 8.0 Hz, $^3J_{PtH}$ = 40 Hz, 1H), 3.88 (s, 3H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 175.1 (C), 166.0 (C), 157.7 (CH), 156.9 (CH), 154.2 (CH), 141.7 (C), 140.4 (C), 140.1 (C), 136.0 (C), 130.5 (CH), 130.2 (CH), 128.5 (CH), 126.6 (CH), 126.1 (CH), 125.4 (CH), 117.3 (CH), 111.7 (CH, $^2J_{PtC}$ = 56.4 Hz,), 55.7 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{22}H_{18}N_3O^{35}C_lNa^{195}Pt$ $[M+Na]^+$: 593.0678, found: 593.0675 (1 ppm).

***Complex 14*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **31** (93 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **14** was obtained as a yellow powder. Yield: 47 % (71 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.89 (dd, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 2.2 Hz, $^3J_{PtH}$ = 36.3 Hz, 1H), 9.06 (d, $^3J_{HH}$ = 4.9 Hz, $^3J_{PtH}$ = 43.2 Hz 2H), 8.78 (dd, $^3J_{HH}$ = 4.7 Hz, $^4J_{HH}$ = 2.2 Hz, 1H), 8.20–8.07 (m, 3H), 7.95 (tt, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 1.6 Hz, 1H), 7.51 (td, $^3J_{HH}$ = 6.5 Hz, $^4J_{HH}$ = 1.5 Hz, 2H), 7.43–7.34 (m, 4H), 7.32–7.24 (m, 3H), 7.18 (t, $^3J_{HH}$ = 5.3 Hz, 1H), 6.63 (d, $^3J_{HH}$ = 8.1 Hz, $^3J_{PtH}$ = 46.2 Hz 1H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): ^{13}C NMR (75 MHz, $CDCl_3$) 163.5 (C), 158.3 (CH), 157.4 (CH), 153.7 (CH), 142.9 (C), 140.6 (C), 139.8 (C), 137.9 (CH), 133.6 (C), 131.3 (CH), 130.7 (CH), 126.0 (CH), 125.9 (CH), 125.6 (C), 123.0 (CH), 120.0 (CH), 119.5 (CH), 117.7 (CH), 109.5 (CH). HRMS (ESI) *m/z* calculated for $C_{27}H_{19}N_4{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 652.0898 ,found: 652.0846 (1 ppm).

***Complex 15*:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **31** (93 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **15** was obtained as a yellow powder. Yield: 70%

(112 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.84 (dd, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 2.2 Hz, $^3J_{PtH}$ = 34 Hz, 1H), 8.82 (d, $^3J_{HH}$ = 7.1 Hz, 2H), 8.71 (dd, $^3J_{HH}$ = 4.8 Hz, $^4J_{HH}$ = 2.3 Hz, 1H), 8.14 (d, $^3J_{HH}$ = 7.7 Hz, 2H), 8.07 (d, $^4J_{HH}$ = 2.4 Hz, 2H), 7.47–7.34 (m, 4H), 7.33–7.21 (m, 3H), 7.11 (t, ^3J = 5.4 Hz, 1H). 6.95 (d, $^3J_{HH}$ = 5.7 Hz, 1H), 6.71 (d, $^3J_{HH}$ = 8.1 Hz, $^3J_{PtH}$ = 40.2 Hz, 1H), 3.92 (s, 3H); $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 174.6 (C), 166.2 (C), 158.1 (CH), 157.2 (CH), 154.1 (CH), 142.0 (C), 140.5 (C), 139.8 (C), 133.3 (C), 131.4 (CH), 130.4 (CH), 125.6 (CH), 122.9 (C), 119.9 (CH), 119.5 (CH), 117.7 (CH), 111.9 (CH), 109.5 (CH), 55.7 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{28}H_{21}N_4O^{35}ClNa^{195}Pt$ $[M+Na]^+$: 682.0944 ,found: 682.0946 (0 ppm).

Complex 16**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **38** (80 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **16** was obtained as a orange powder. Yield: 65 % (110 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.79 (dd, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 2.1 Hz, $^3J_{PtH}$ = 35.4 Hz, 1H), 9.15 (dd, $^3J_{HH}$ = 5.0 Hz, $^4J_{HH}$ = 1.6 Hz, $^3J_{PtH}$ = 41.1 Hz, 2H), 8.68 (s, 1H), 8.05–7.90 (m, 2H), 7.73 (d, $^3J_{HH}$ = 7.7 Hz, 1H), 7.56–7.40 (m, 3H), 7.38–7.29 (m, 1H), 7.09 (t, $^3J_{HH}$ = 7.5 Hz, 1H), 7.02–6.92 (m, 2H), 4.38 (q, $^3J_{HH}$ = 7.2 Hz, 2H), 1.43 (t, $^3J_{HH}$ = 7.2 Hz, 3H). $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 175.8 (C), 157.8 (CH), 157.2 (CH), 154.0 (CH), 140.8 (C), 138.2 (C), 137.6 (CH), 137.4 (C), 128.6 (C), 126.6 (C), 126.3 (CH), 125.7 (CH, $^2J_{PtC}$ = 51.6 Hz), 121.9(C), 121.1 (CH), 120.7 (CH), 118.4 (CH), 116.8 (CH), 108.5 (CH), 107.9 (CH), 37.3 (CH_2), 13.6 (CH_3). HRMS (ESI) *m/z* calculated for $C_{23}H_{19}N_4{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 604.0838, found: 604.0835 (0 ppm).

Complex 17: Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **32** (54 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **17** was obtained as a orange powder. Yield: 15 % (20 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.60 (d, $^3J_{HH}$ = 3.3 Hz, $^4J_{HH}$ = 1.2 Hz, $^3J_{PtH}$ = 22,5 Hz, 1H), 9.08–8.84 (m, 3H), 8.33 (d, $^3J_{HH}$ = 3.3 Hz, 1H), 7.92 (t, $^3J_{HH}$ = 7.7 Hz, 1H), 7.53–7.41 (m, 2H), 7.12 (d, $^4J_{HH}$ = 2.7 Hz, 2H), 6.70 (dd, $^3J_{HH}$ = 8.4, $^4J_{HH}$ = 2.7 Hz, 1H), 6.25 (d, $^3J_{HH}$ = 8.4 Hz, $^3J_{PtH}$ = 44.4 Hz, 1H), 3.81 (s, 3H). $^{13}C\{1H\}$ NMR (JMOD, 75 MHz, $CDCl_3$): 156.7 (C), 153.6 (CH), 143.8 (CH), 143.5 (CH), 142.4 (C), 140.8 (CH), 137.9 (CH), 133.8 (C), 131.5 (CH, $^2J_{PtC}$ = 71 Hz), 125.9 (CH, $^2J_{PtC}$ = 51.6 Hz), 120.3 (C), 117.1 (CH), 109.5 (CH, $^2J_{PtC}$ =46.2 Hz), 55.2(OCH_3).HRMS (ESI) *m/z* calculated for $C_{16}H_{14}N_3O^{35}ClNa^{195}Pt$ $[M+Na]^+$: 517.0365, found: 517.0371 (1 ppm).

Complex 18**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **34** (94 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **18** was obtained as a orange powder. Yield: 17 % (25 mg). NMR (δ (ppm), $CDCl_3$): ^1H (300 MHz): 9.66 (dd, $^3J_{HH}$ = 3.3 Hz, $^5J_{HH}$ = 1.3 Hz, $^3J_{PtH}$

= 38.7 Hz, 1H), 8.97 (d, $^3J_{HH}$ = 6.6 Hz, $^3J_{PtH}$ = 42.3 Hz, 2H), 8.76 (s, 1H), 8.36 (d, $^3J_{HH}$ = 3.3 Hz, 1H), 7.91 (tt, $^3J_{HH}$ = 7.8 Hz, $^4J_{HH}$ = 1.6 Hz, 1H), 7.46 (td, $^3J_{HH}$ = 6.5 Hz, $^4J_{HH}$ = 1.5 Hz, 2H), 7.39 (d, $^4J_{HH}$ = 2.4 Hz, 1H), 7.29–7.19 (m, 4H), 7.13–7.05 (m, 4H), 7.04–6.95 (m, 2H), 6.87 (dd, $^3J_{HH}$ = 8.3 Hz, $^4J_{HH}$ = 2.4 Hz, 1H), 6.29 (d, $^3J_{HH}$ = 8.3 Hz, $^3J_{PtH}$ = 44.1 Hz, 1H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 161.0 (C), 153.6 (CH), 147.3 (C), 144.2 (C), 143.7 (CH), 143.4 (CH), 142.8 (C), 141.0 (CH), 137.9 (CH), 137.3 (C), 131.7 (CH, $^2J_{PtC}$ = 68 Hz), 129.0 (CH), 128.1 (CH), 125.9 (CH, $^2J_{PtC}$ = 54 Hz), 123.3 (CH), 122.3 (CH), 120.6 (CH). HRMS (ESI) *m/z* calculated for $C_{27}H_{21}N_4{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 654.0994, found: 654.0991(1 ppm).

Complex 19**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **33** (68 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **19** was obtained as an orange powder. Yield: 13 % (17 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 9.68 (d, $^3J_{HH}$ = 3.4 Hz, $^5J_{HH}$ = 1.1 Hz, $^3J_{PtH}$ = 40.8 Hz, 1H), 9.14–8.85 (m, 3H), 8.40 (d, $^3J_{HH}$ = 3.4 Hz, 1H), 7.95 (t, $^3J_{HH}$ = 7.8 Hz, 1H), 7.78 (d, $^4J_{HH}$ = 2.0 Hz, 1H), 7.65–7.55 (m, 2H), 7.54–7.27 (m, 6H), 6.47 (d, $^3J_{HH}$ = 8.1 Hz, $^3J_{PtH}$ = 43.2 Hz, 1H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 155.2(C), 153.6(CH), 145.9(CH), 144.9(CH), 142.3(C), 134.0(C), 134.5(C), 131.0(CH), 129.7(CH), 129.5(CH), 128.7(CH), 127.6(CH), 127.0(CH), 126.4(CH), 125.8(CH), 122.5(CH). HRMS (ESI) *m/z* calculated for $C_{21}H_{16}N_3{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 563.0573, found: 563.0583 (2 ppm).

Complex 20**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **35** (93 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **20** was obtained as a yellow powder. Yield: 16 % (25 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): ^{1}H NMR (300 MHz, $CDCl_3$) 9.75 (dd, $^3J_{HH}$ = 3.3 Hz, $^5J_{HH}$ = 1.3 Hz, $^3J_{PtH}$ = 39.6 Hz, 1H), 9.03 - 8.94 (m, 3H), 8.47 (d, $^3J_{HH}$ = 3.3 Hz, 1H), 8.15 (d, $^3J_{HH}$ = 7.7 Hz, 2H), 7.98 (t, $^3J_{HH}$ = 7.8 Hz, 1H), 7.78 (d, $^4J_{HH}$ = 2.2 Hz, 1H), 7.60–7.48 (m, 2H), 7.45–7.28 (m, 7H), 6.64 (d, $^3J_{HH}$ = 7.9 Hz, $^3J_{PtH}$ = 45 Hz, 1H).^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 153.6 (CH), 149.1 (C), 146.9 (CH),144.1(CH), 143.9 (CH), 142.6 (C), 141.0 (CH), 140.7 (C), 138.2 (CH), 133.6 (C), 132.7 (CH), 132.2 (CH), 130.8 (C), 129.9 (CH), 126.1 (CH), 125.7 (CH), 123.0 (C), 122.6 (CH), 120.1 (CH), 119.7 (CH), 109.3 (CH); HRMS (ESI) *m/z* calculated for $C_{27}H_{19}N_4{}^{35}ClNa^{195}Pt$ $[M+Na]^+$: 652.0838, found: 652.0848 (2 ppm).

Complex 21**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **36** (70 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **21** was obtained as a red powder. Yield: 35% (56 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 10.28 (s, $^3J_{PtH}$ = 20.1 Hz, 1H), 9.04 (dd, $^3J_{HH}$ =

6.3 Hz, $^4J_{HH}$ = 1.5 Hz, $^3J_{PtH}$ = 45.9 Hz, 2H), 8.71 (d, $^3J_{HH}$ = 8.1 Hz, 1H), 8.21–8.02 (m, 1H), 8.02–7.89 (m, 2 H), 7.79–7.67 (m, 2 H), 7.53–7.41 (m, 2H), 6.79 (dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 2.7 Hz, 1H), 6.42 (d, $^3J_{HH}$ = 8.5 Hz, $^3J_{PtH}$ = 31.8 Hz, 1H), 3.83 (s, 3H). ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 156.0 (C), 153.7 (CH), 151.1 (C), 148.5 (C), 144.6 (C), 138.5 (CH), 137.7 (C), 134.9 (CH), 131.6 (CH), 129.2 (CH), 128.4 (CH), 125.9 (CH), 125.5 (CH), 124.4 (CH), 120.5 (C), 118.2 (CH), 117.2 (CH), 55.4 (OCH_3). HRMS (ESI) *m/z* calculated for $C_{20}H_{16}N_3O^{35}ClNa^{195}Pt$ $[M+Na]^+$: 567.0522, found: 567.0522 (0 ppm).

Complex 22**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **36** (70 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **22** was obtained as a red powder. Yield: 45% (64 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 10.20 (s, 1H), 8.84 (d, $^3J_{HH}$ = 5.7 Hz, $^3J_{PtH}$ = 42.9 Hz, 2H), 8.62 (d, $^3J_{HH}$ = 8.6 Hz, 1H), 8.05 (d, $^3J_{HH}$ = 8.6 Hz, 1H), 7.92 (t, $^3J_{HH}$ = 6.9 Hz, 1H), 7.69 (t, $^3J_{HH}$ = 8.4 Hz, 1H), 7.58 (d, $^4J_{HH}$ = 2.7 Hz, 1H), 6.95 (d, $^3J_{HH}$ = 7.1 Hz, 2H), 6.68 (dd, $^3J_{HH}$ = 9.1 Hz, $^4J_{HH}$ = 3.2 Hz, 1H), 6.43 (d, $^3J_{HH}$ = 8.5 Hz, $^3J_{PtH}$ = 54.6 Hz, 1H), 3.95 (s, 3H), 3.75 (s, 3H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 166.1 (C), 155.9 (C), 154.1 (CH), 150.9 (C), 137.6 (C), 134.7 (CH), 131.6 (CH), 129.4 (C), 128.3 (CH), 128.2 (CH), 125.4 (CH), 117.8 (CH), 117.7 (C), 116.9 (CH), 116.0 (C), 111.8 (CH), 55.8 (CH_3), 55.2 (OCH_3). HRMS (ESI) *m/z* calculated for $C_{21}H_{18}N_3O_2^{35}ClNa^{195}Pt$ $[M+Na]^+$: 597.0627, found: 597.0627 (0 ppm).

Complex 23**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **37** (109 mg, 0.29 mmol) and pyridine (48 mg, 0.05 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The complex **23** was obtained as a violet powder. Yield: 75 % (123 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 10.28 (s, 1H), 9.03 (d, $^3J_{HH}$ = 6.3 Hz, $^4J_{HH}$ = 1.5 Hz, $^3J_{PtH}$ = 47.4 Hz, 2H), 8.20 (d, $^3J_{HH}$ = 7.8 Hz, 1H), 8.06 (d, $^3J_{HH}$ = 7.2 Hz, 1H), 7.97–7.81 (m, 3H), 7.53–7.40 (m, 3H), 7.31–7.21 (m, 4H), 7.18–7.09 (m, 4H), 7.06–6.92 (m, 3H), 6.42 (d, $^3J_{HH}$ = 8.4 Hz, $^3J_{PtH}$ = 45 Hz, 1H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 153.7 (CH), 153.1 (CH), 151.0 (C), 147.4 (C), 144.6 (C), 143.8 (C), 137.8 (CH), 134.8 (CH), 134.3 (C), 132.2 (C), 131.7 (CH), 129.7 (CH), 128.3 (CH), 127.6 (CH), 125.9 (CH), 125.5 (CH), 124.1 (CH), 122.5 (CH), 120,3 (C); HRMS (ESI) *m/z* calculated for $C_{31}H_{23}N_4^{35}ClNa^{195}Pt$ $[M+Na]^+$: 704.1151, found: 704.1149 (0 ppm).

Complex 24**:** Synthesized from K_2PtCl_4 (100 mg, 0.24 mmol), ligand **37** (109 mg, 0.29 mmol) and 4-methoxypyridine (66 mg, 0.07 ml, 0.6 mmol) following the general procedure for the synthesis of Pt^{II} complexes. The product **24** was obtained as a blue/violet powder. Yield: 65% (112 mg). NMR (δ (ppm), $CDCl_3$): ^{1}H (300 MHz): 10.27 (s, 1H), 8.79 (d, $^3J_{HH}$ = 5.7 Hz, $^3J_{HH}$ = 1.2 Hz, $^3J_{PtH}$ = 44.4 Hz, 2H), 8.19 (d, $^3J_{HH}$ = 7.7 Hz, 1H), 8.05 (d, $^3J_{HH}$ = 8.6 Hz, 1H), 7.91–7.82 (m, 2H), 7.56 –7.42 (t, $^3J_{HH}$ = 8.4 Hz, 1H), 7.32–7.20 (m, 4H), 7.18–7.10 (m, 4H), 7.05–6.89 (m, 5H), 6.51 (d, $^3J_{HH}$ = 8.4 Hz, $^3J_{PtH}$ = 38.4 Hz, 1H), 3.95 (s, 3H); ^{13}C{1H} NMR (JMOD, 75 MHz, $CDCl_3$): 166.3 (C), 154.1 (CH),150.9 (C), 147.4 (C), 144.7 (C), 143.9 (C), 139.8 (CH), 134.7 (CH), 133.4 (C), 132.5 (C), 131.1 (CH), 129.1 (CH), 128.3 (CH), 127.6 (CH), 125.4 (CH), 123.4 (CH), 122.4 (CH), 121.0 (C), 111.9 (CH), 55.8 (OCH_3); HRMS (ESI) *m/z* calculated for $C_{32}H_{25}N_4O^{195}Pt$ $[M+Na]^+$: 676.1670 ,found: 676.1670 (0 ppm).

NMR spectra

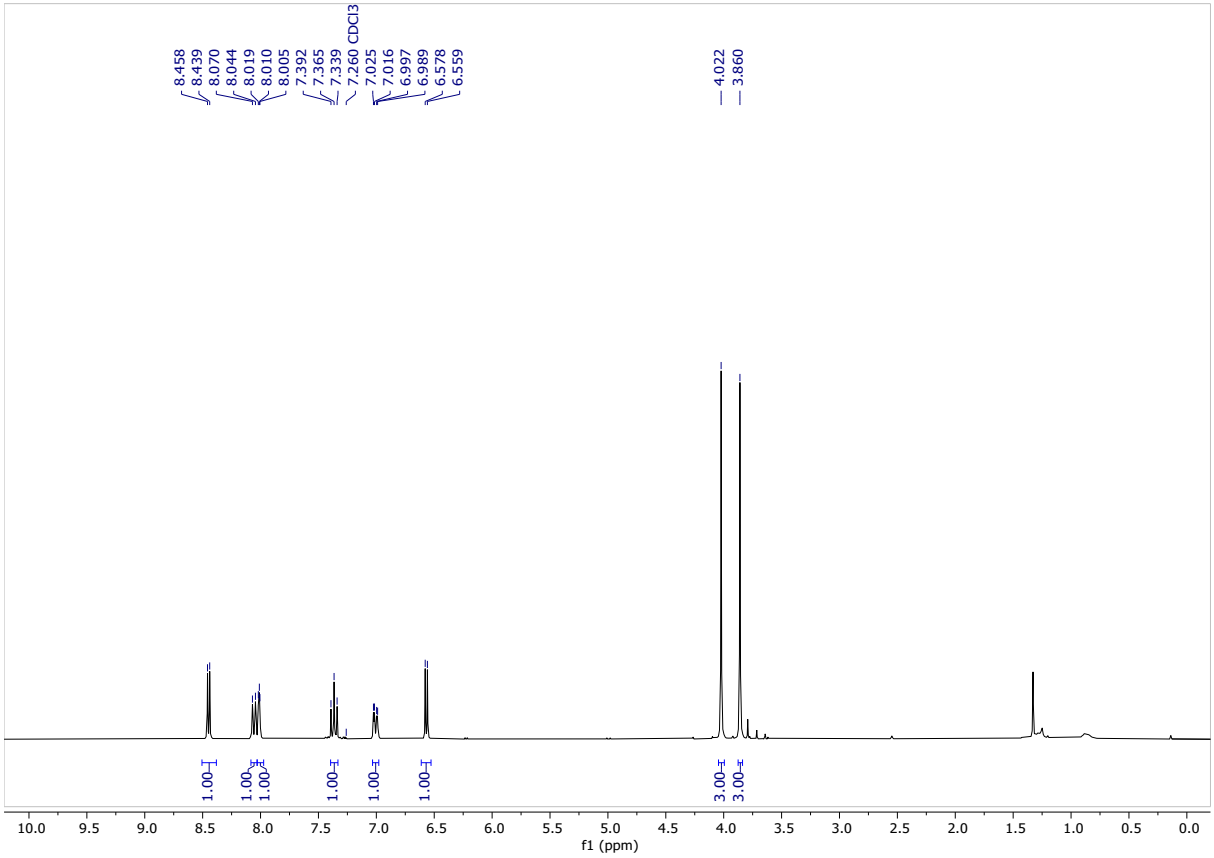


Fig. S1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **26**.

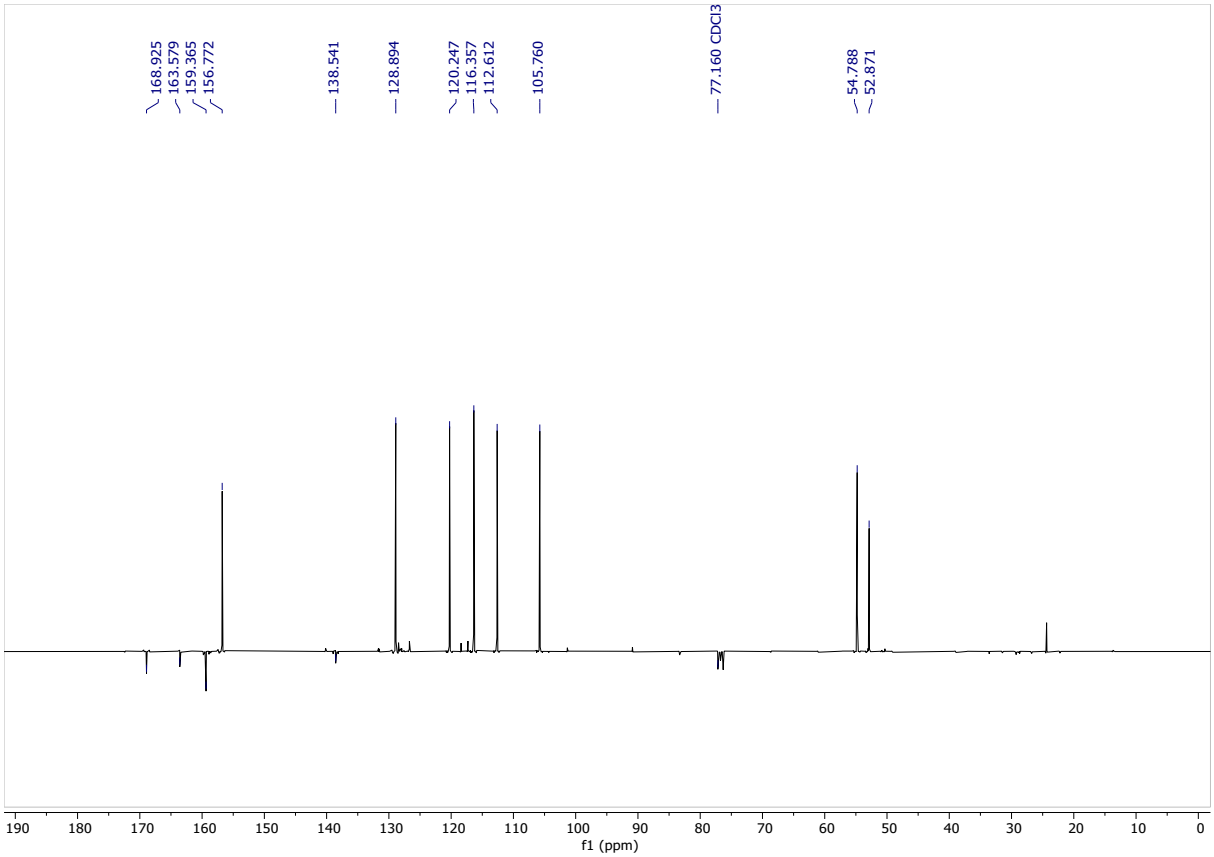


Fig. S2. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **26**.

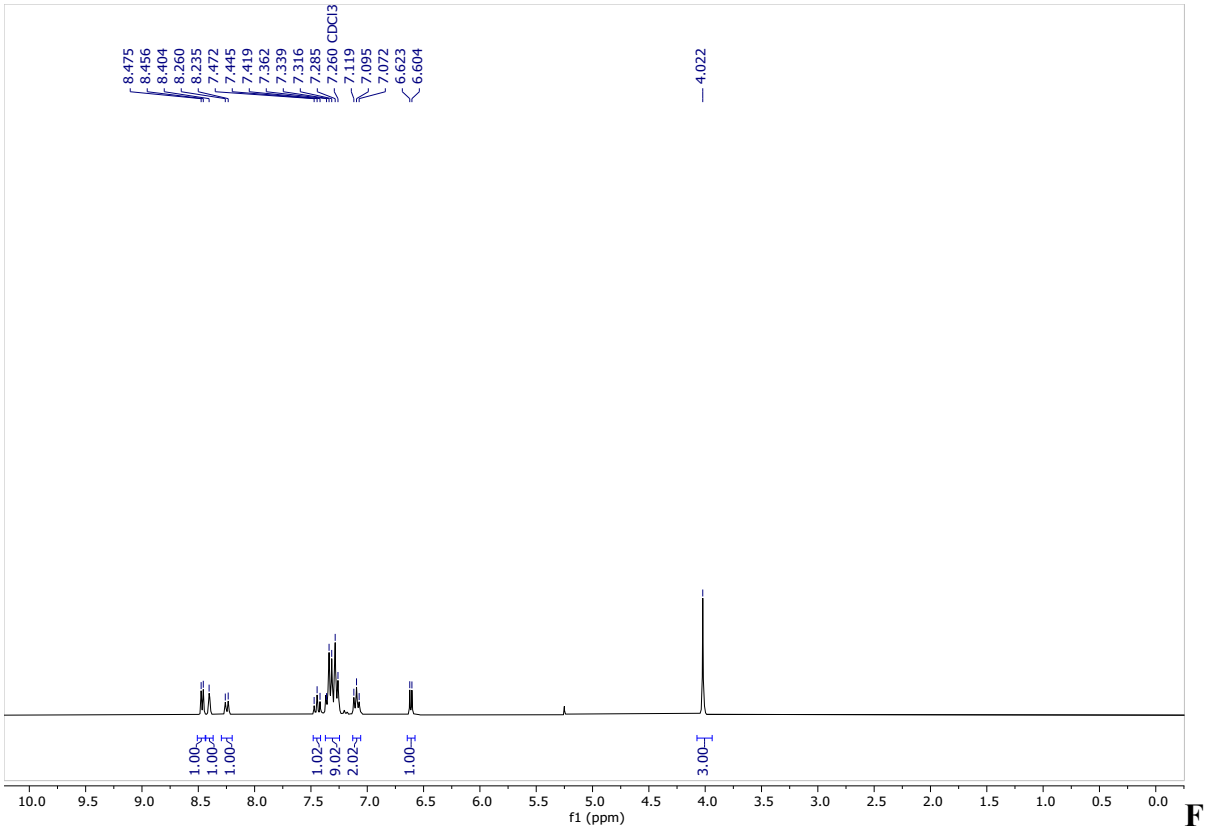


Fig. S3. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **29**.

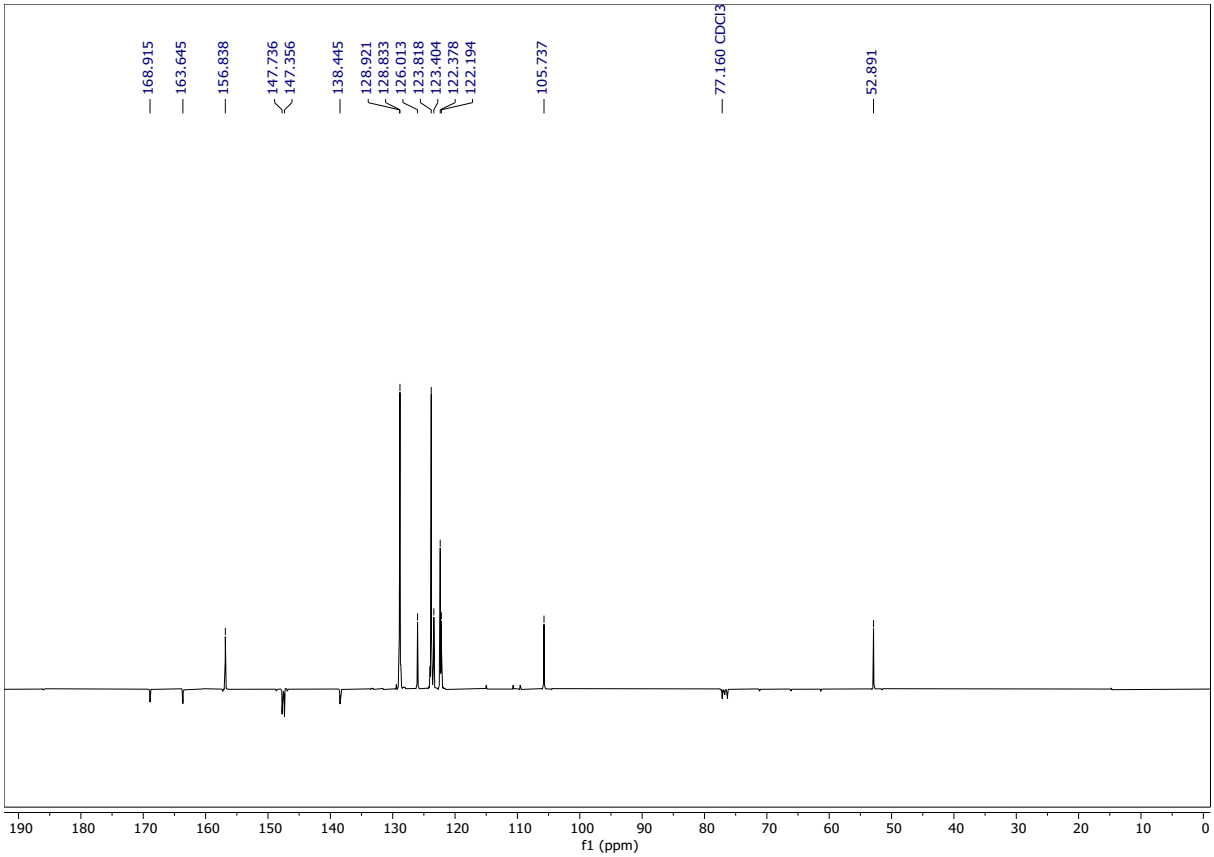


Fig. S4. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **29**.

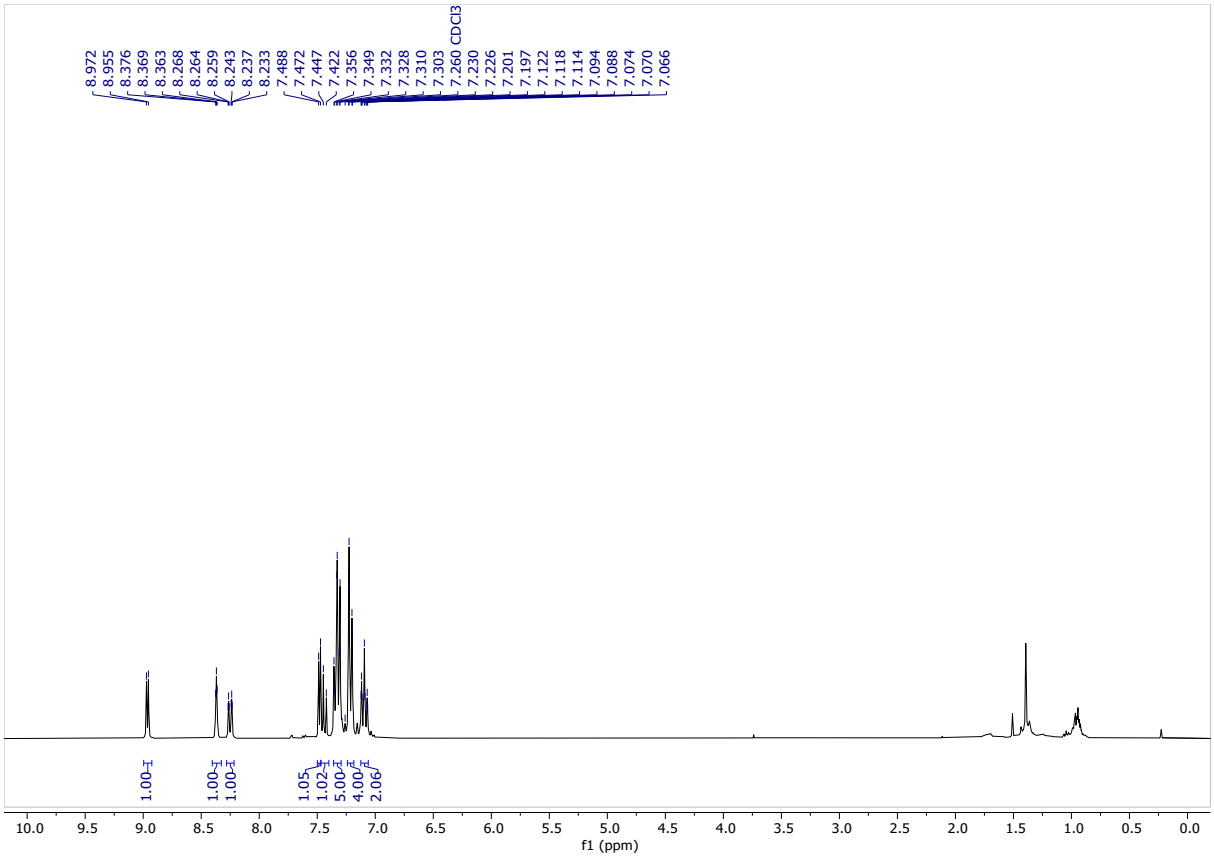


Fig. S5. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **30**.

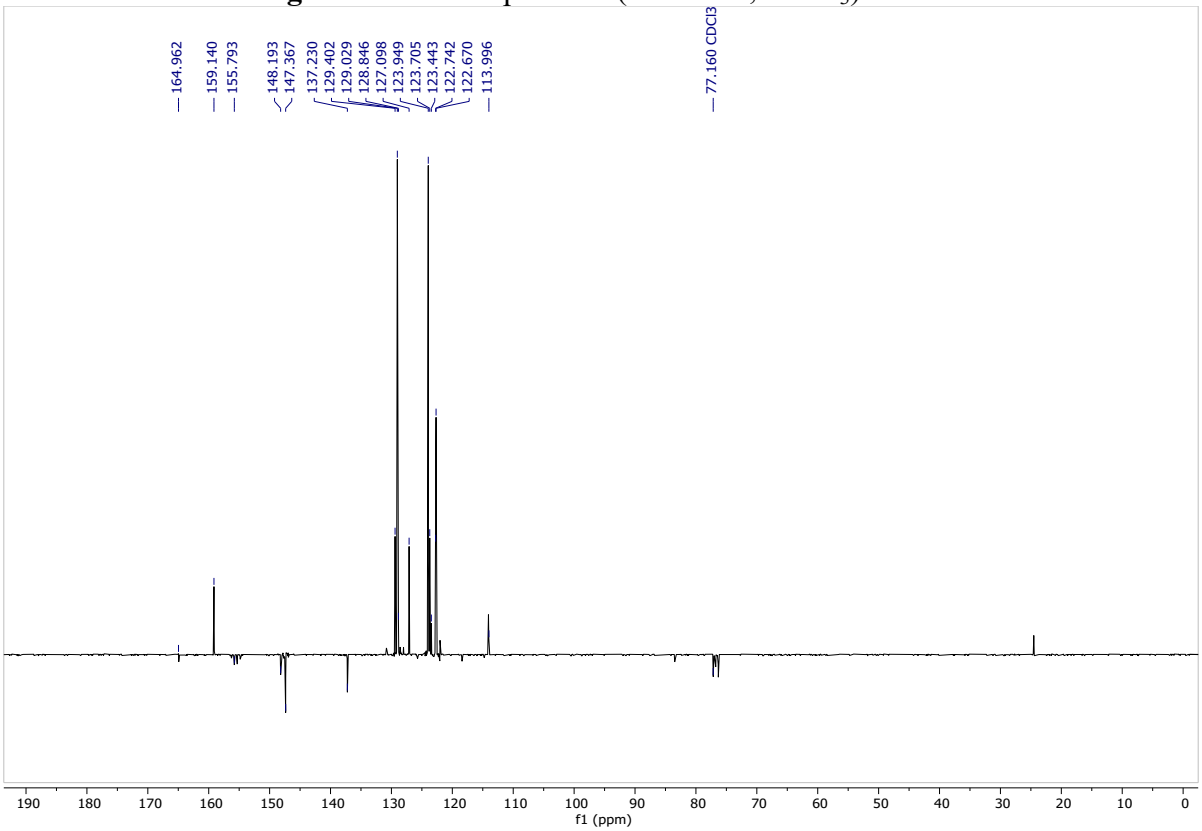
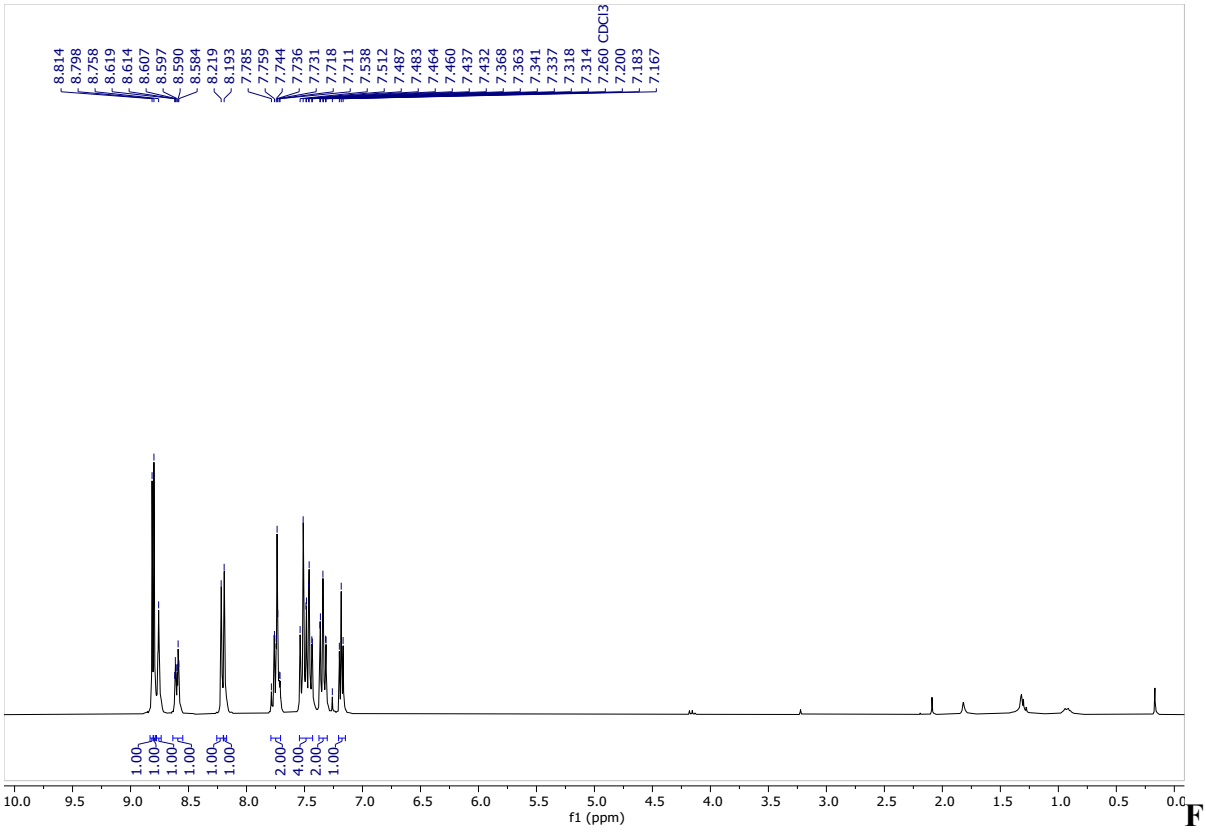


Fig. S6. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **30**.



ig. S7. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **31**.

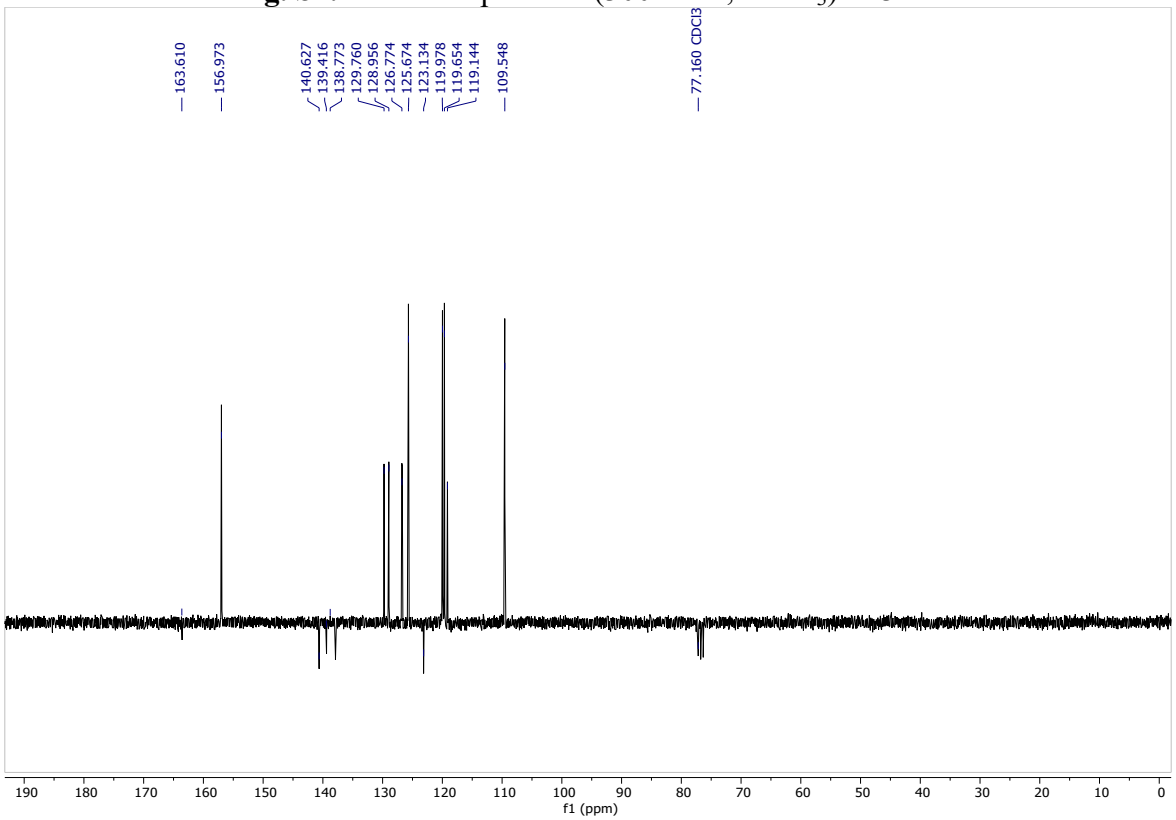


Fig. S8. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **31**.

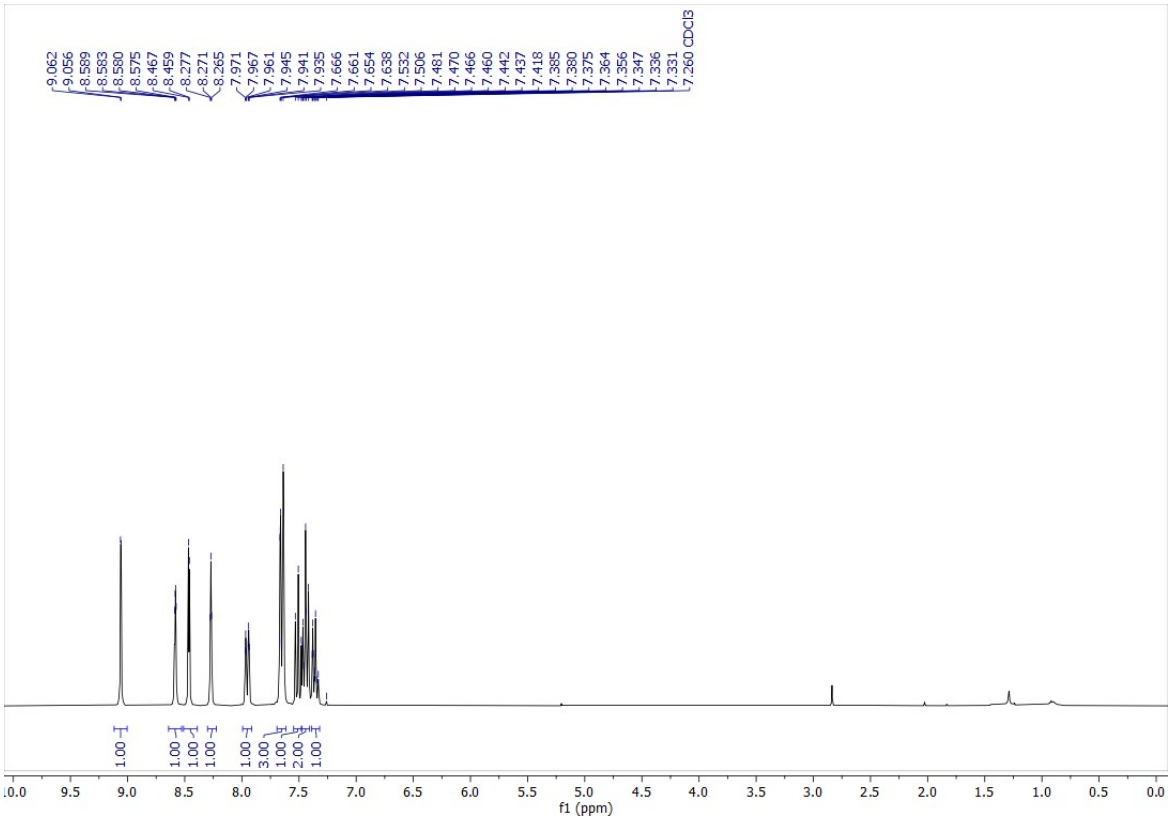


Fig. S9. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **33**.

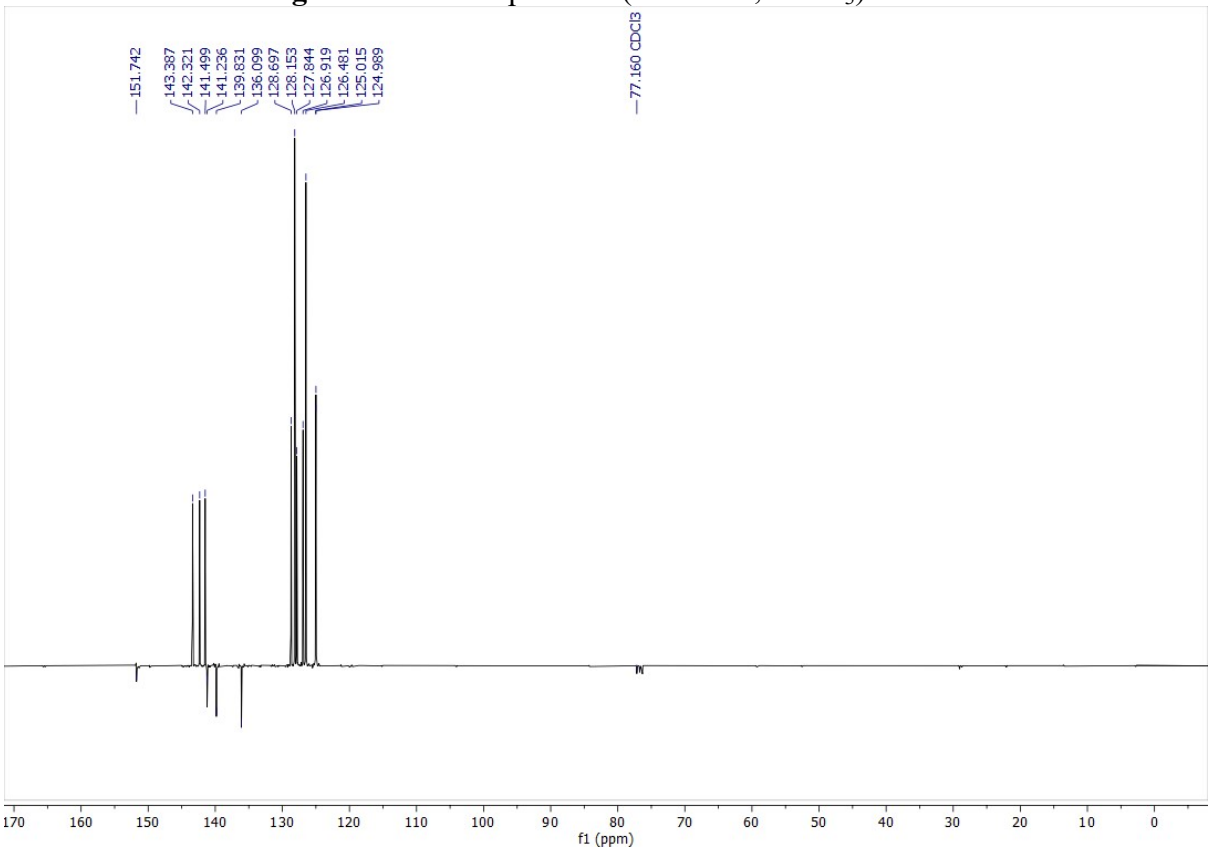


Fig. S10.^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **33**.

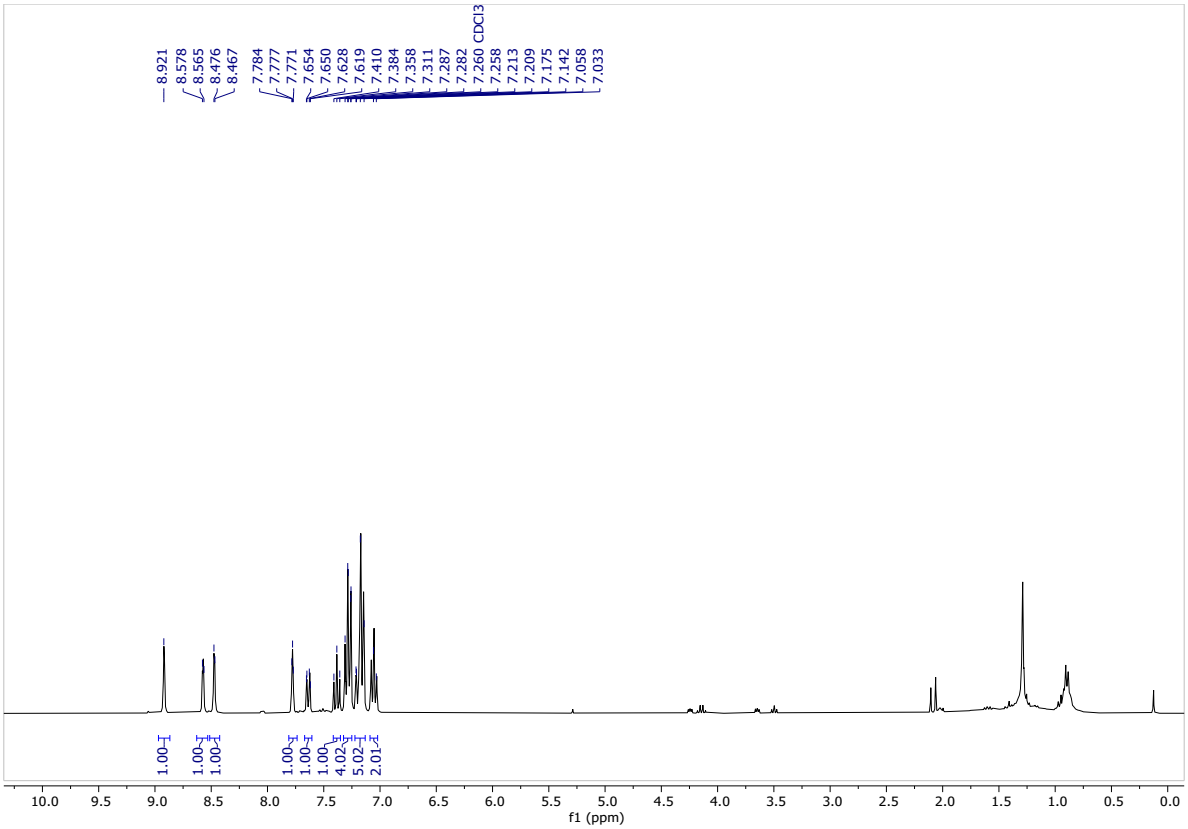


Fig. S11. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **34**.

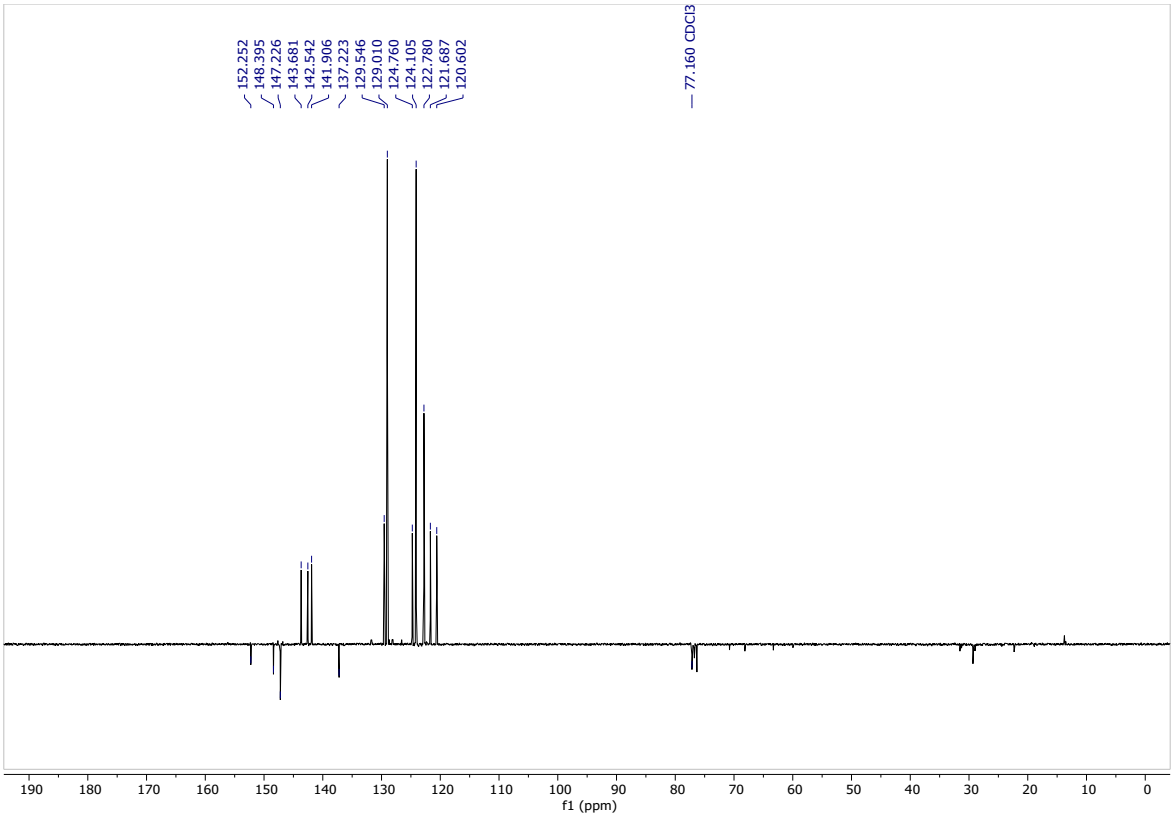


Fig. S12. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **34**.

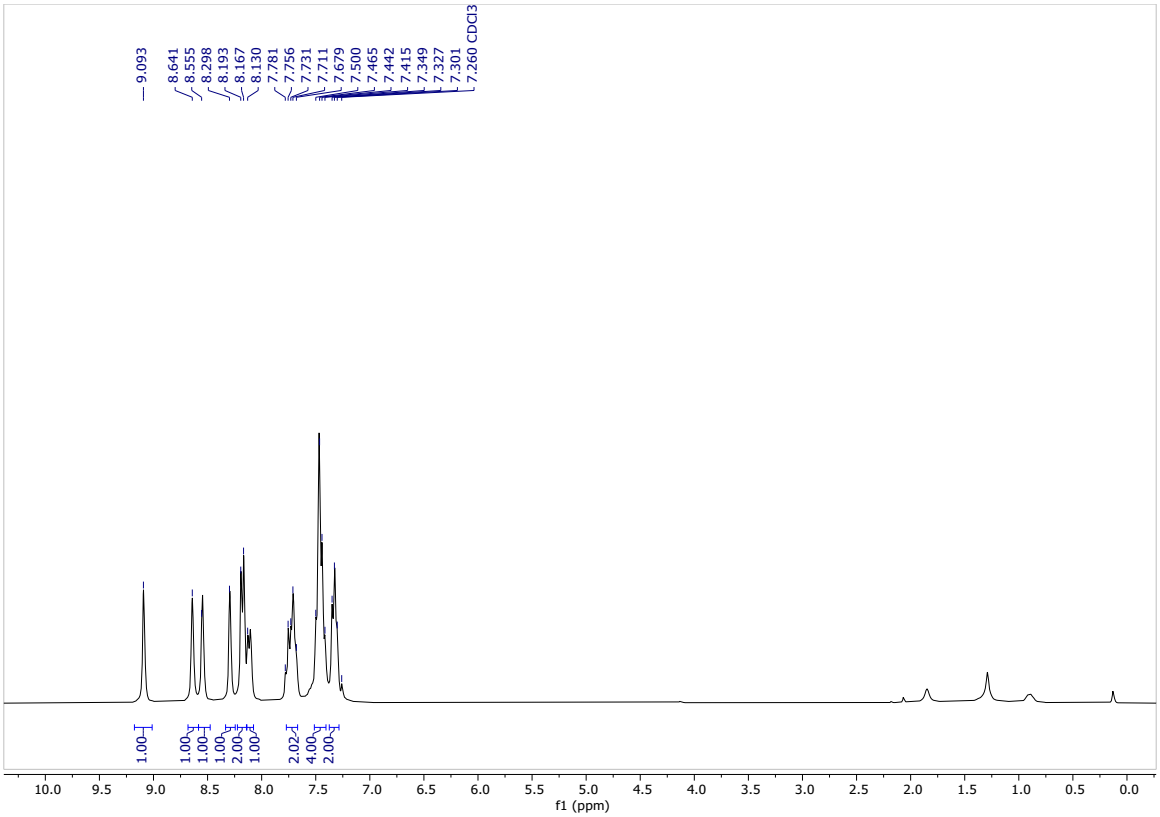


Fig. S13. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **35**.

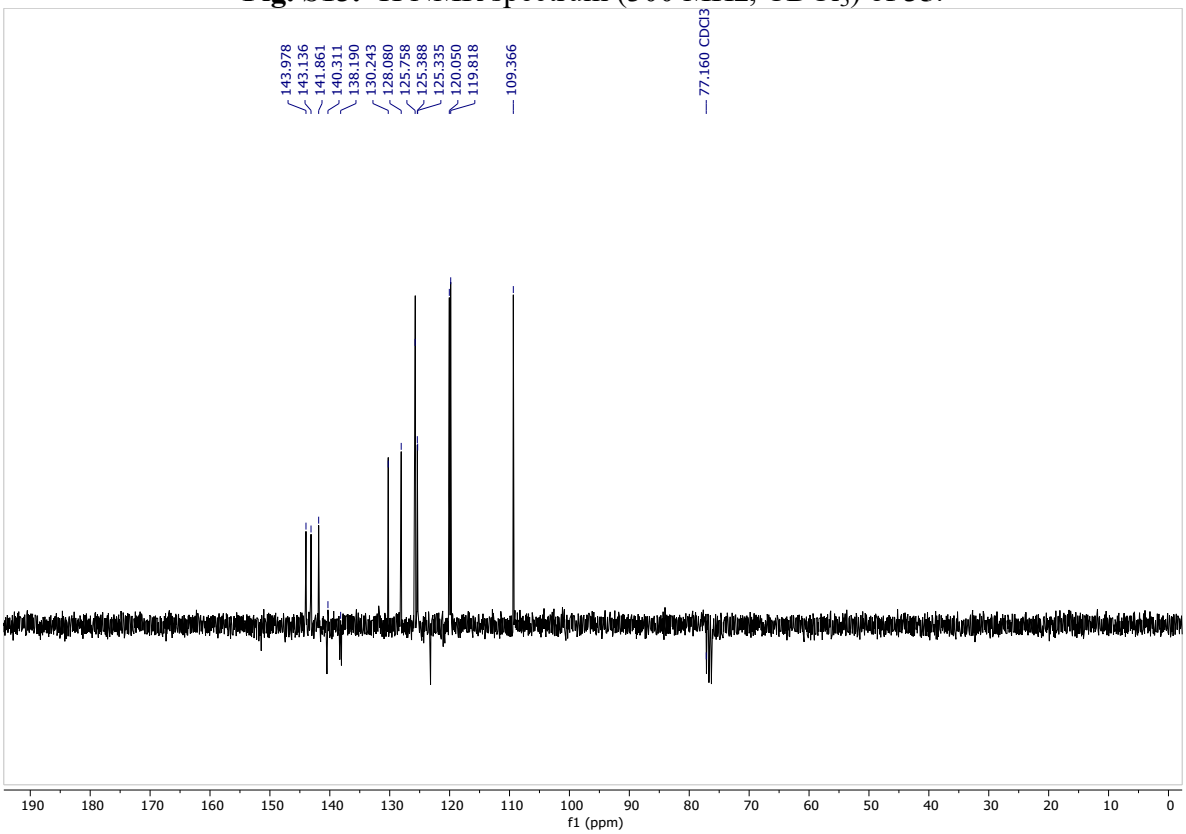


Fig. S14. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **35**.

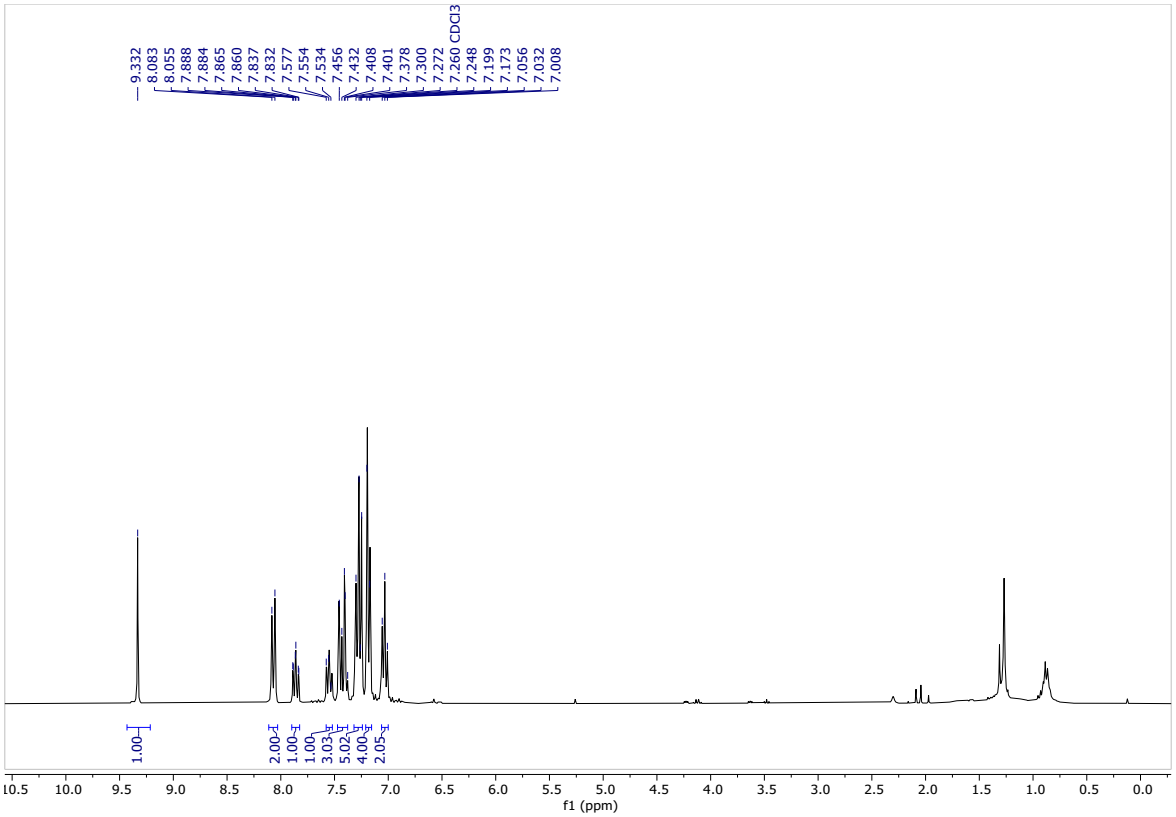


Fig. S15. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **37**.

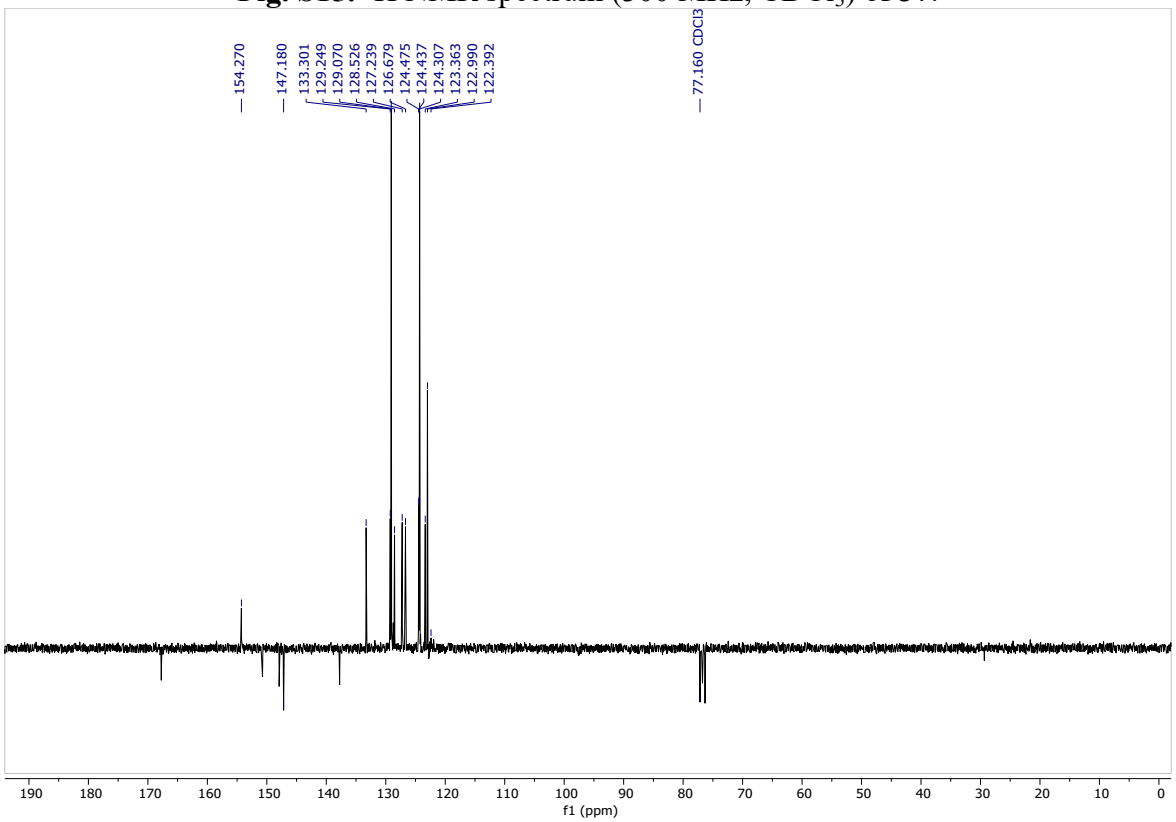


Fig. S16. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **37**.

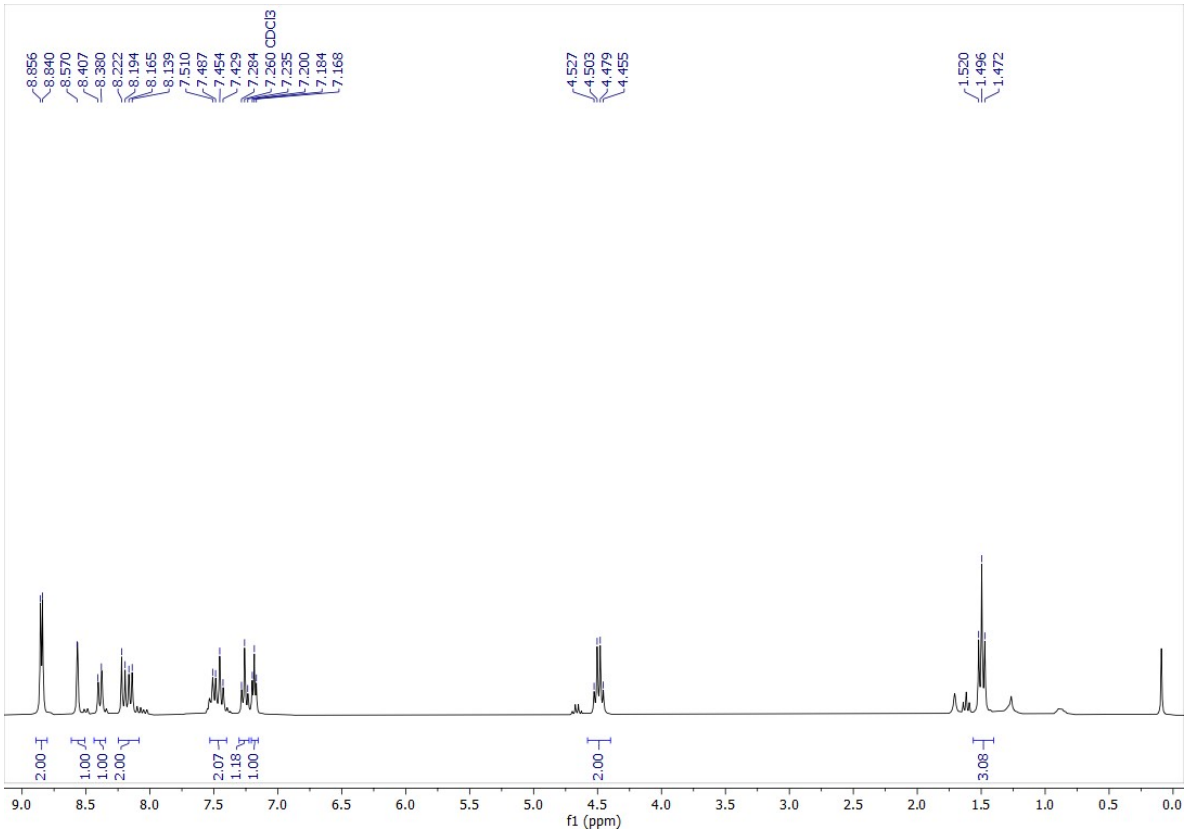


Fig. S17. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **38**.

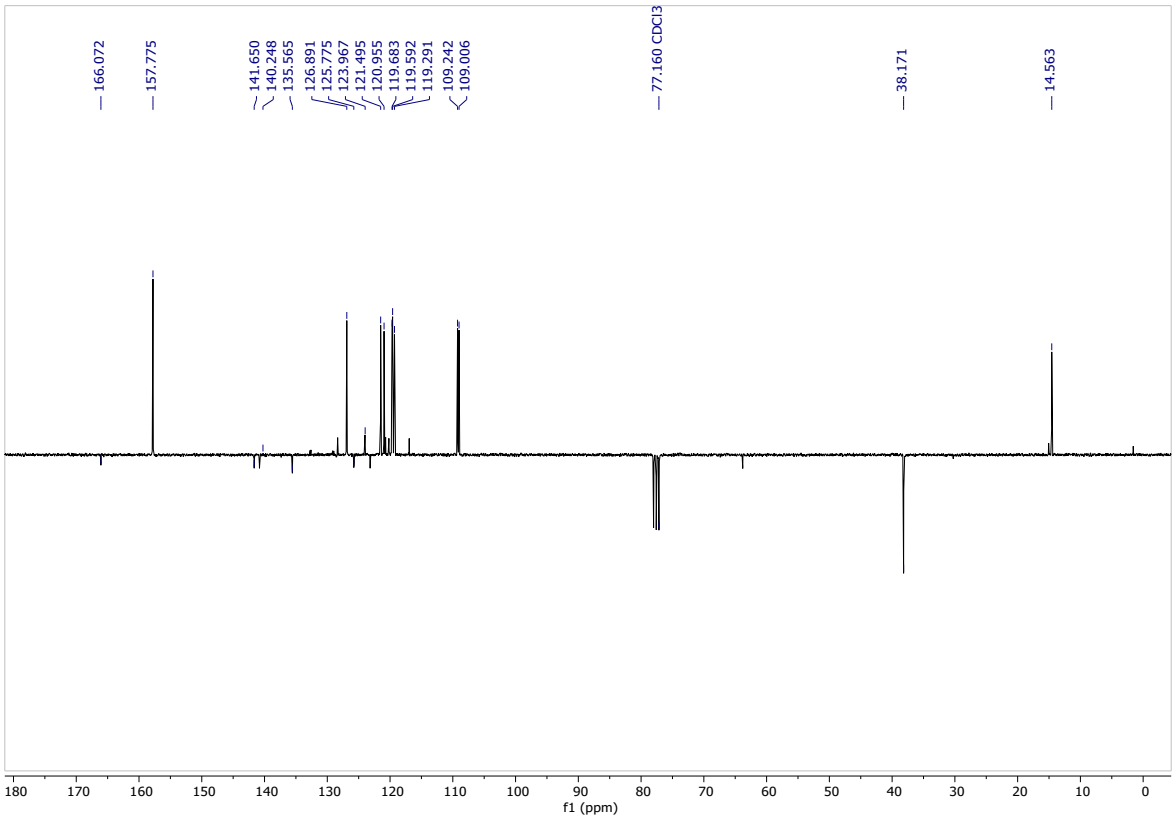


Fig. S18. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **38**.

Complex **2**

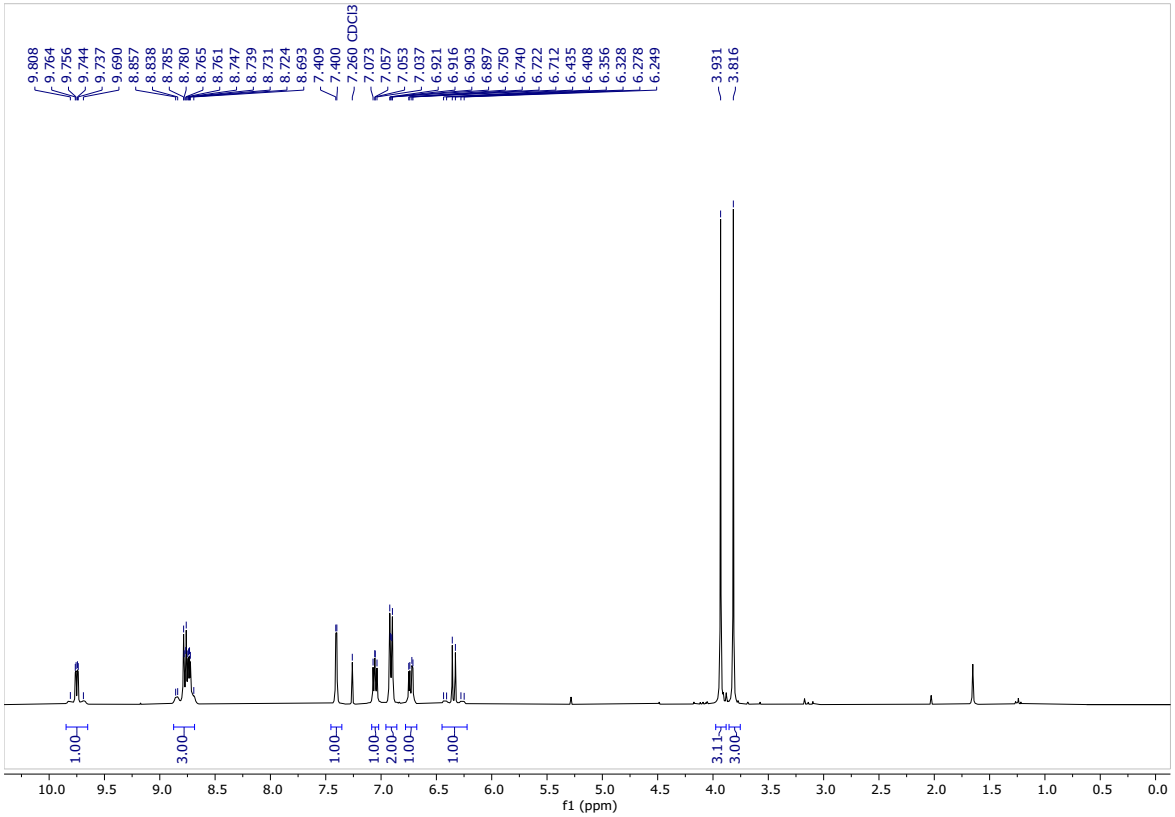


Fig. S19. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **2**.

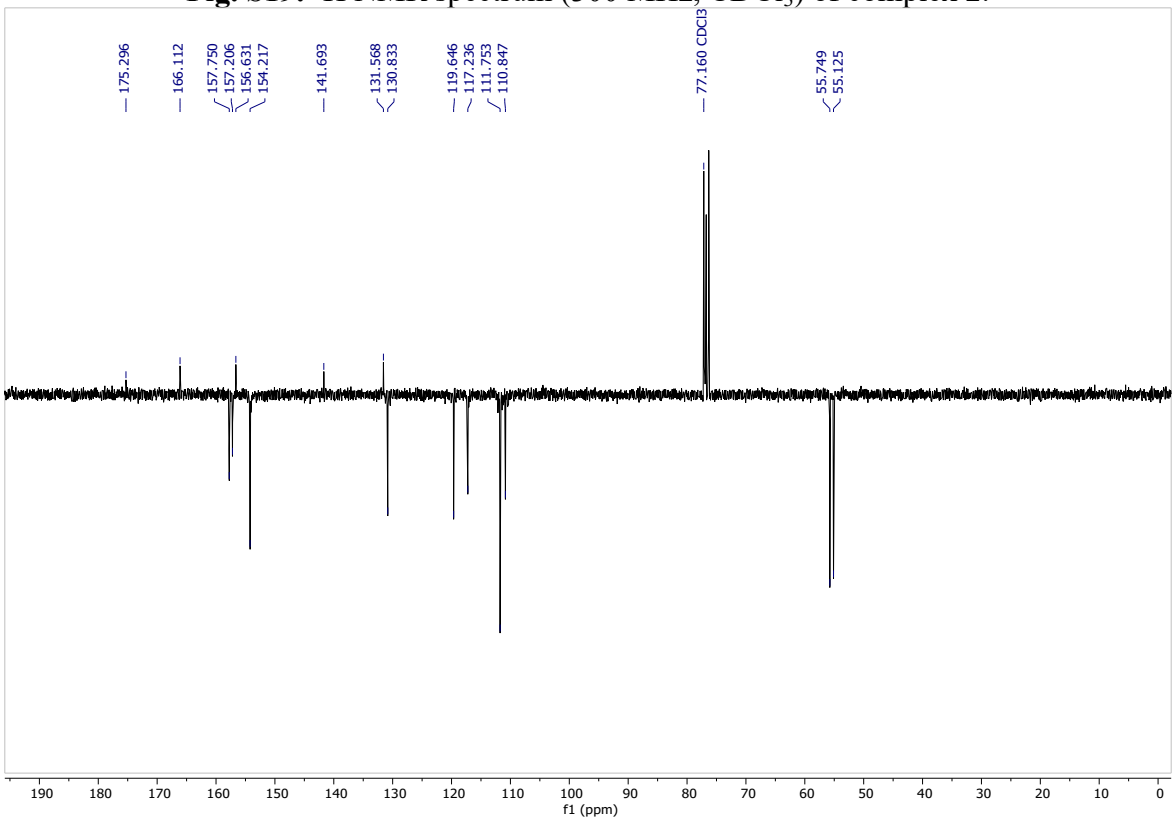


Fig. S20. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **2**.

Complex **3**

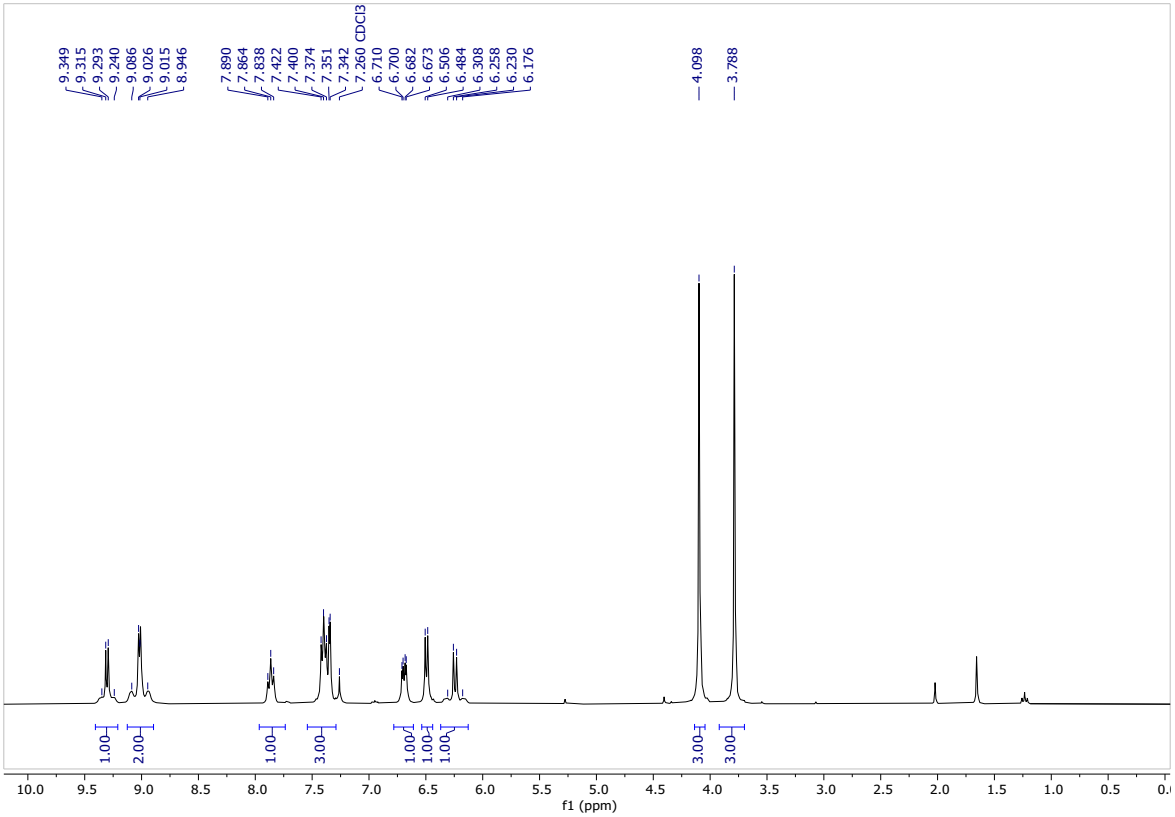


Fig. S21. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **3**.

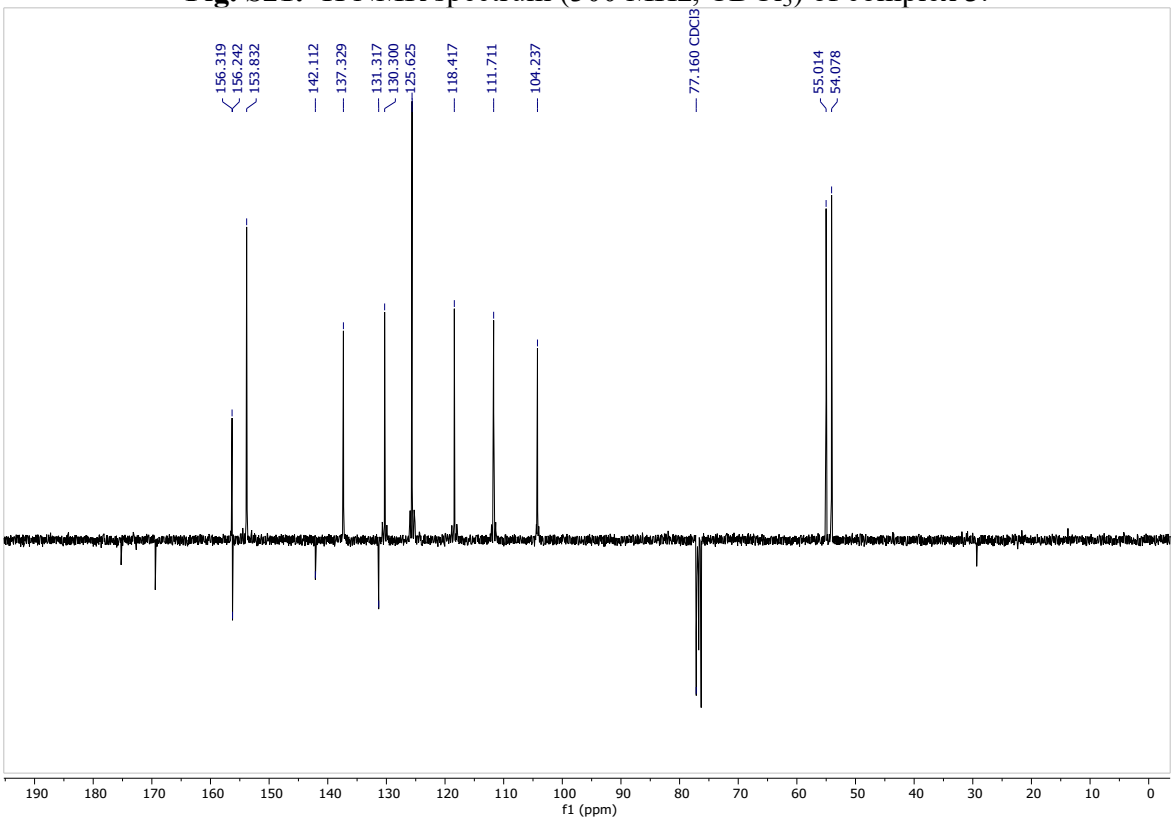


Fig. S22. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **3**.

Complex **4**

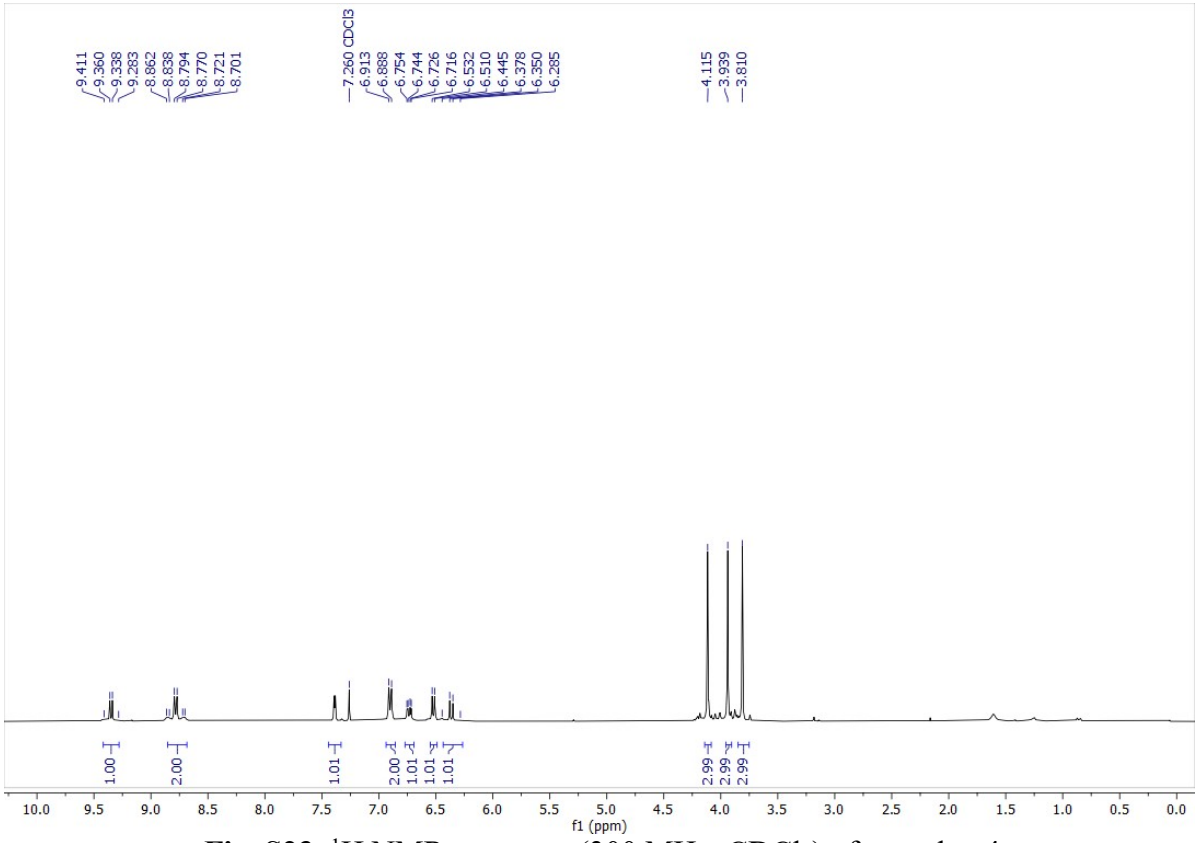


Fig. S23. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **4**.

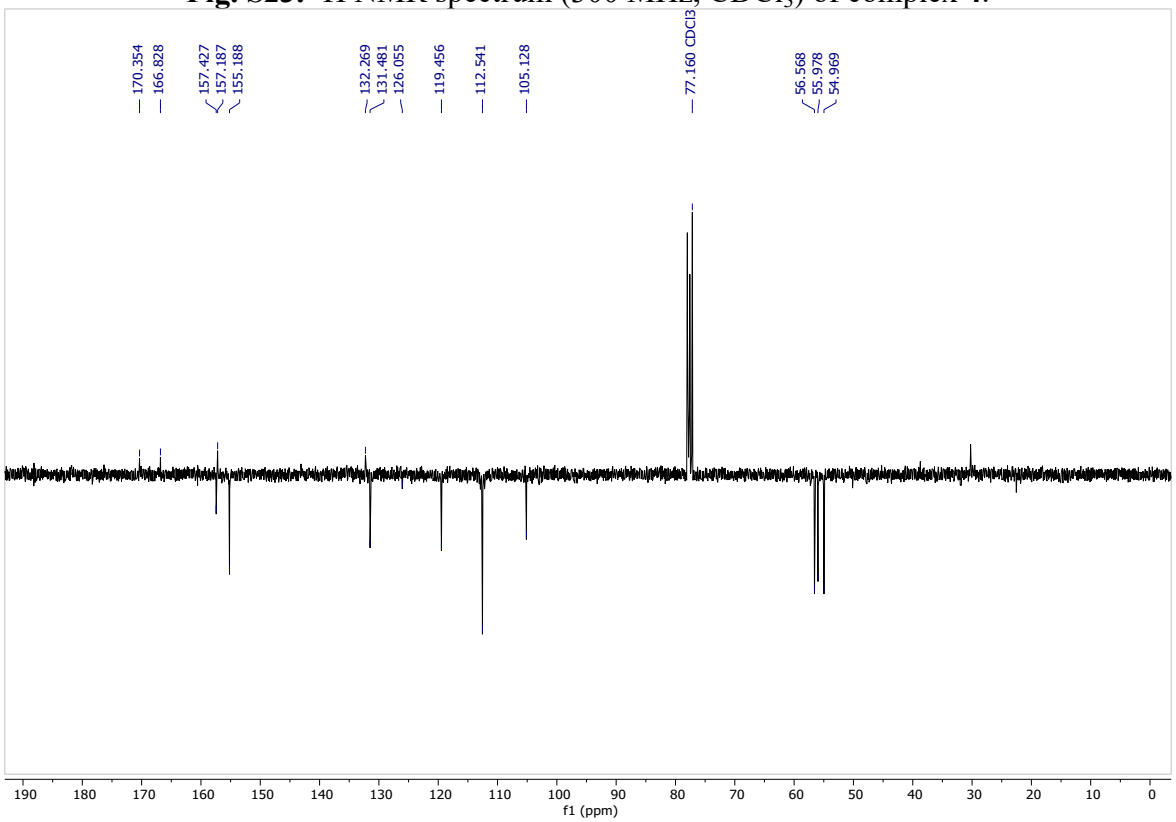


Fig. S24. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **4**.

Complex **5**

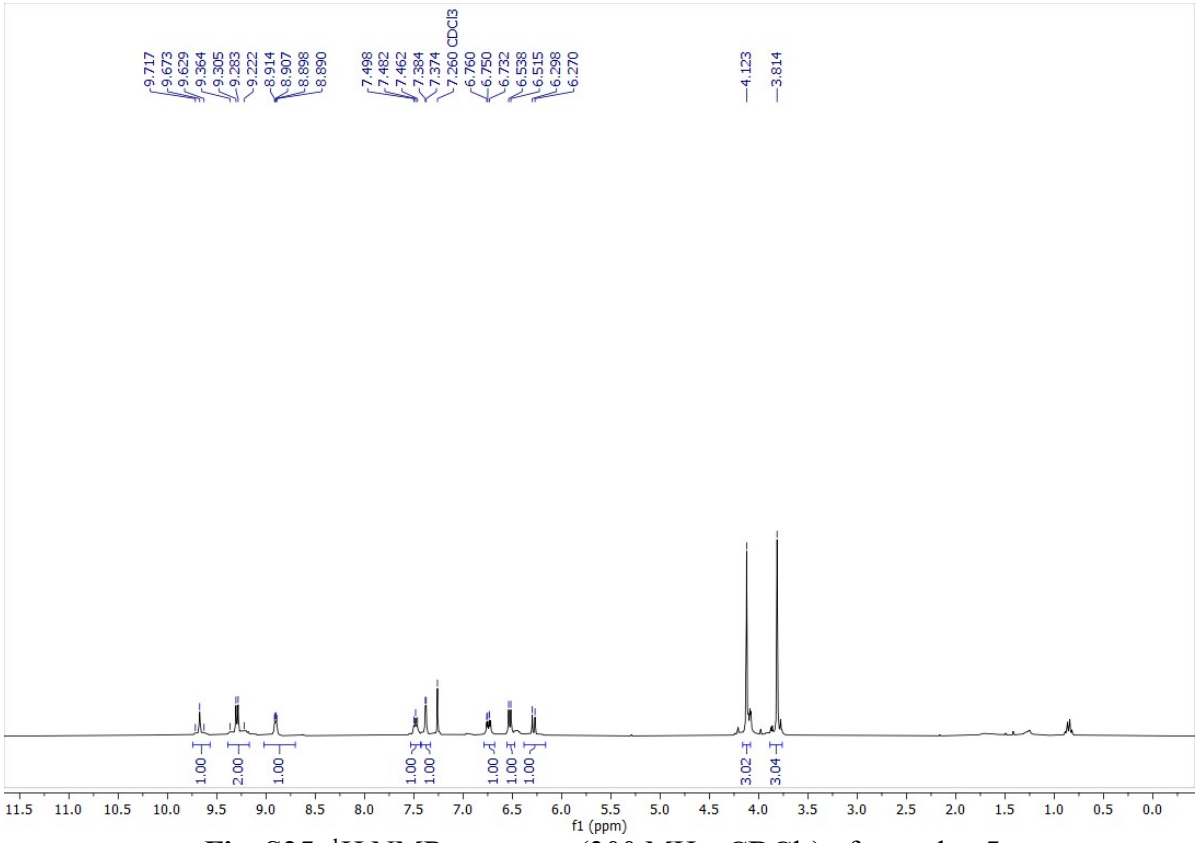


Fig. S25. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **5**.

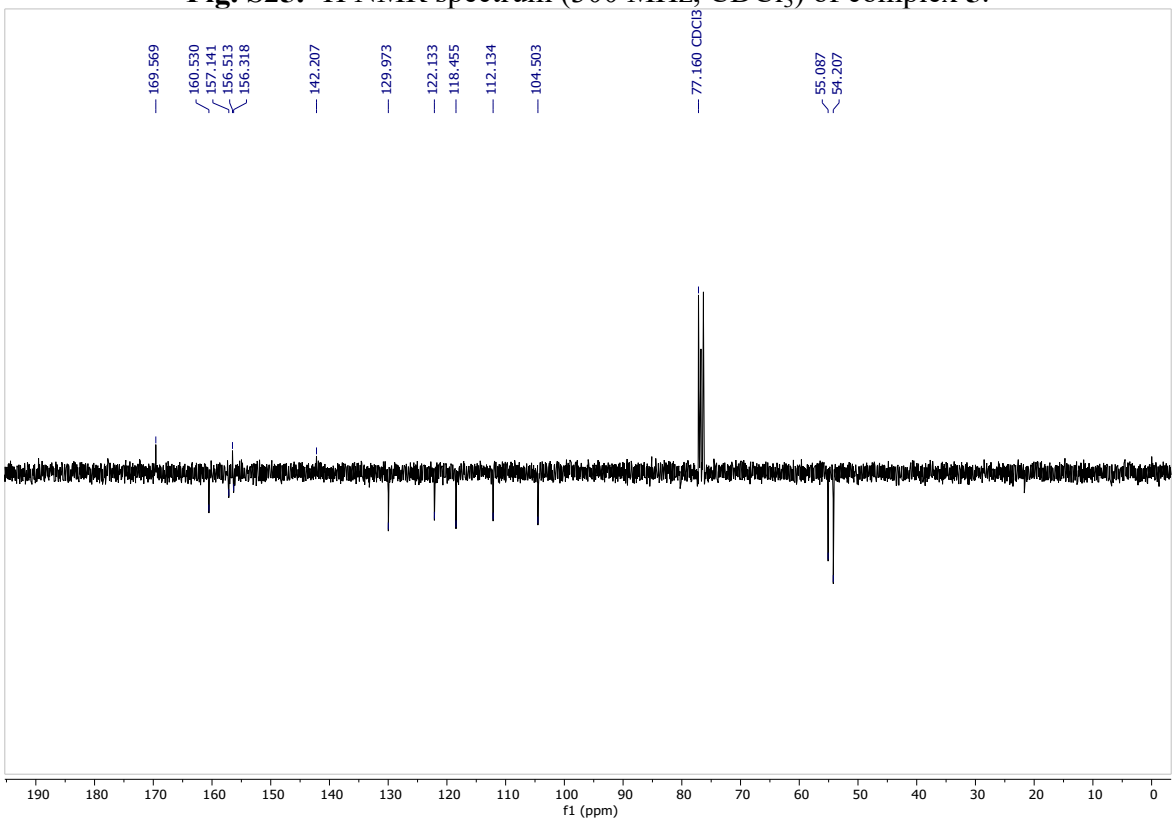


Fig. S26. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **5**.

Complex **7**

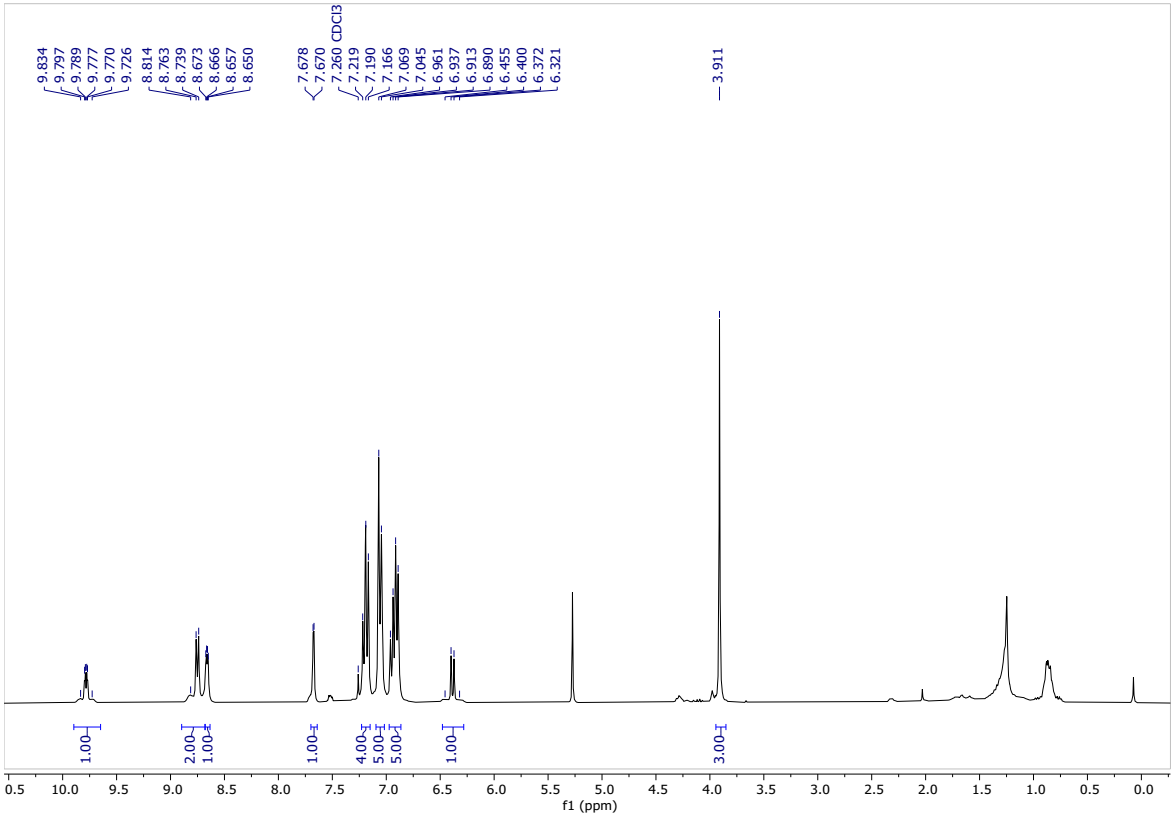


Fig. S27. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **7**.

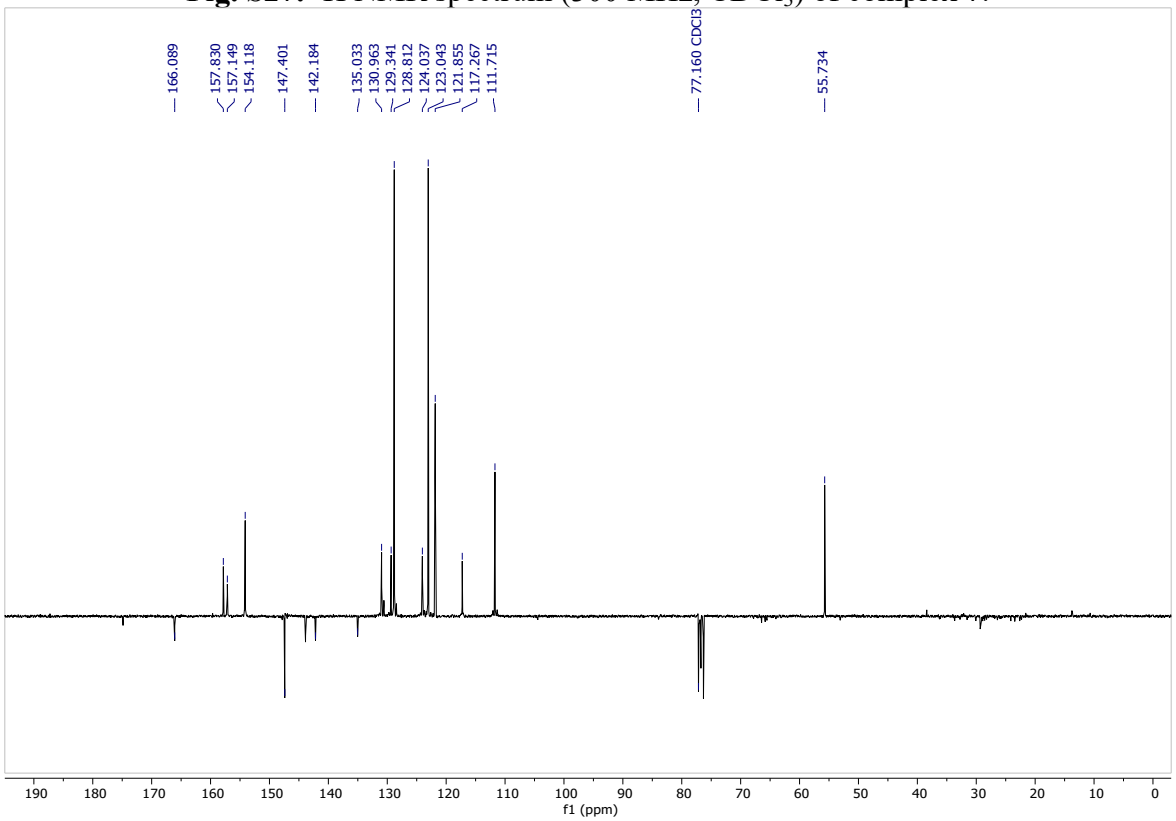


Fig. S28. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **7**.

Complex **8**

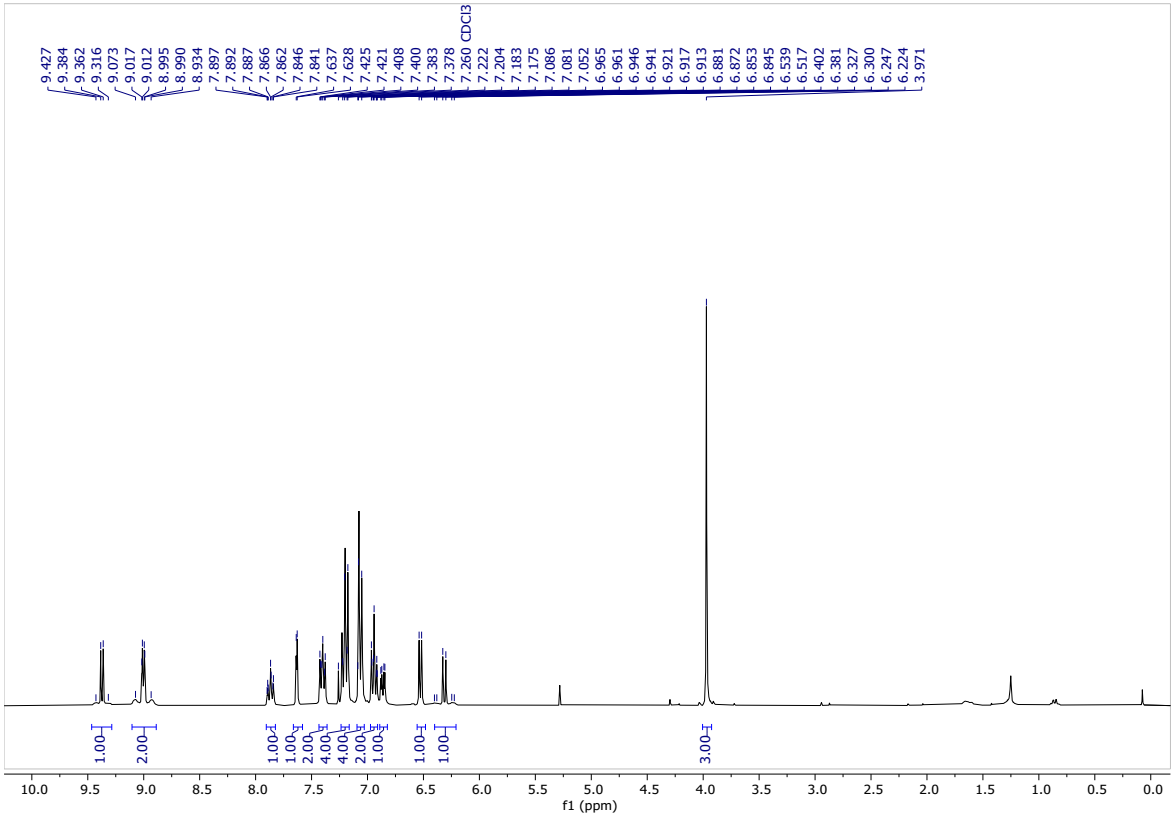


Fig. S29. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **8**.

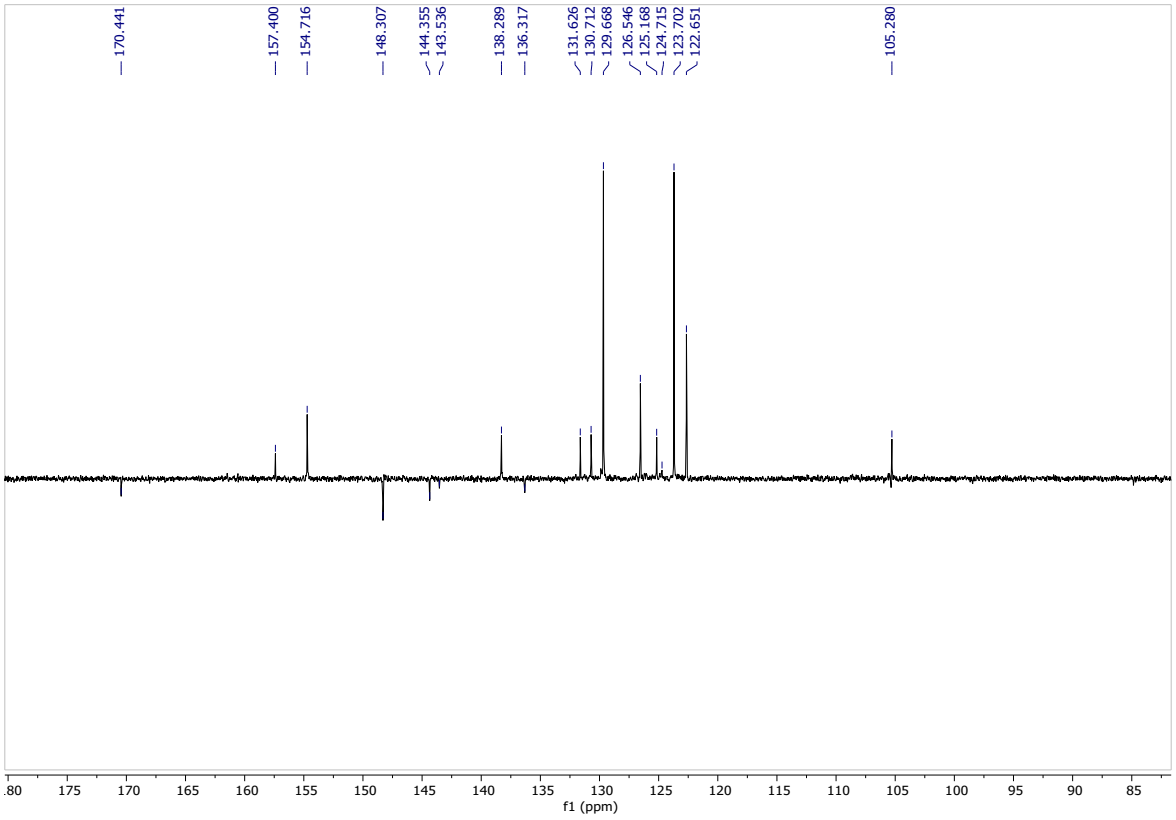


Fig. S30. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **8**.

Complex **9**

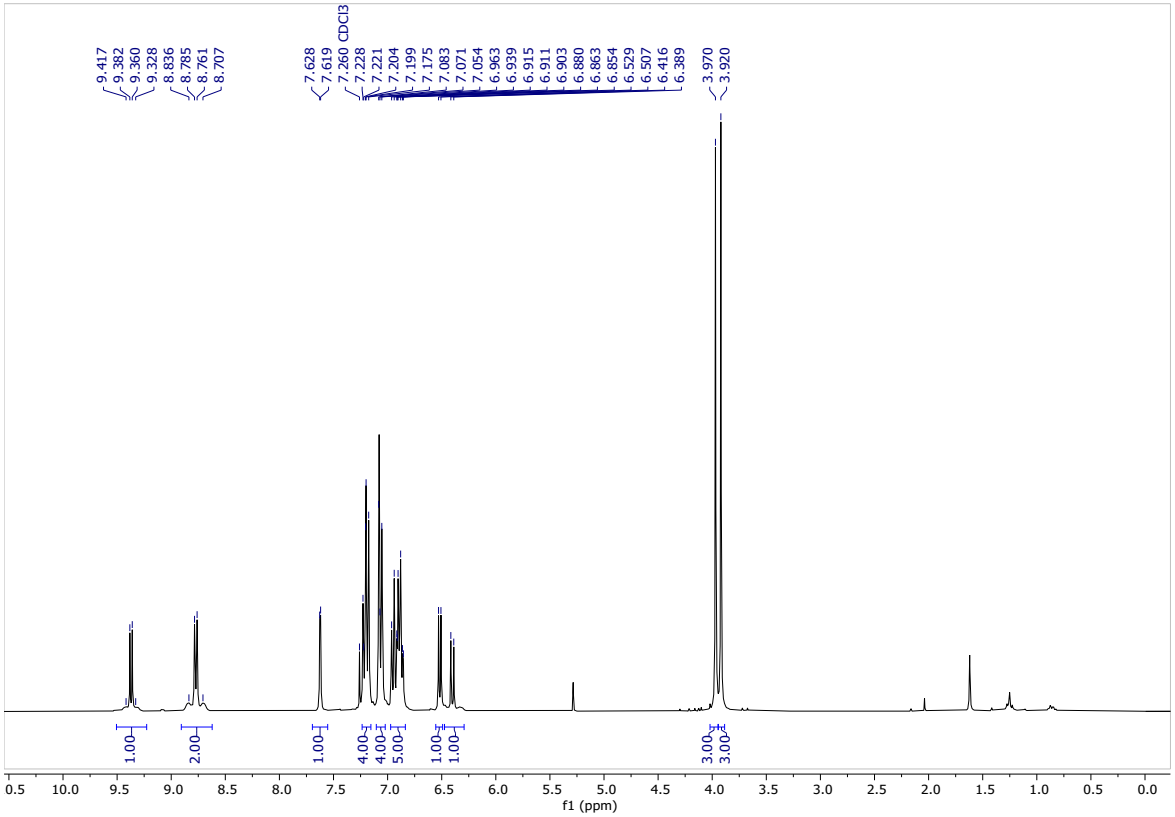


Fig. S21. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **9**.

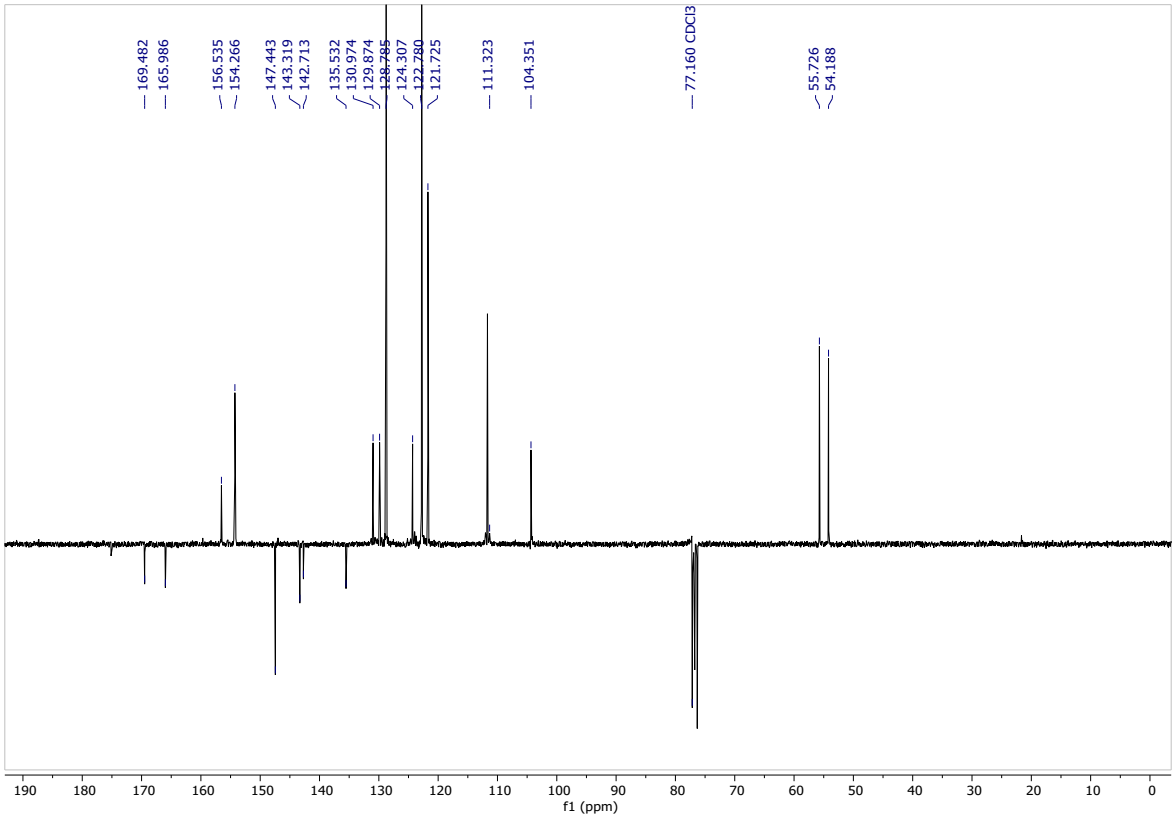


Fig. S32. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **9**.

Complex **10**

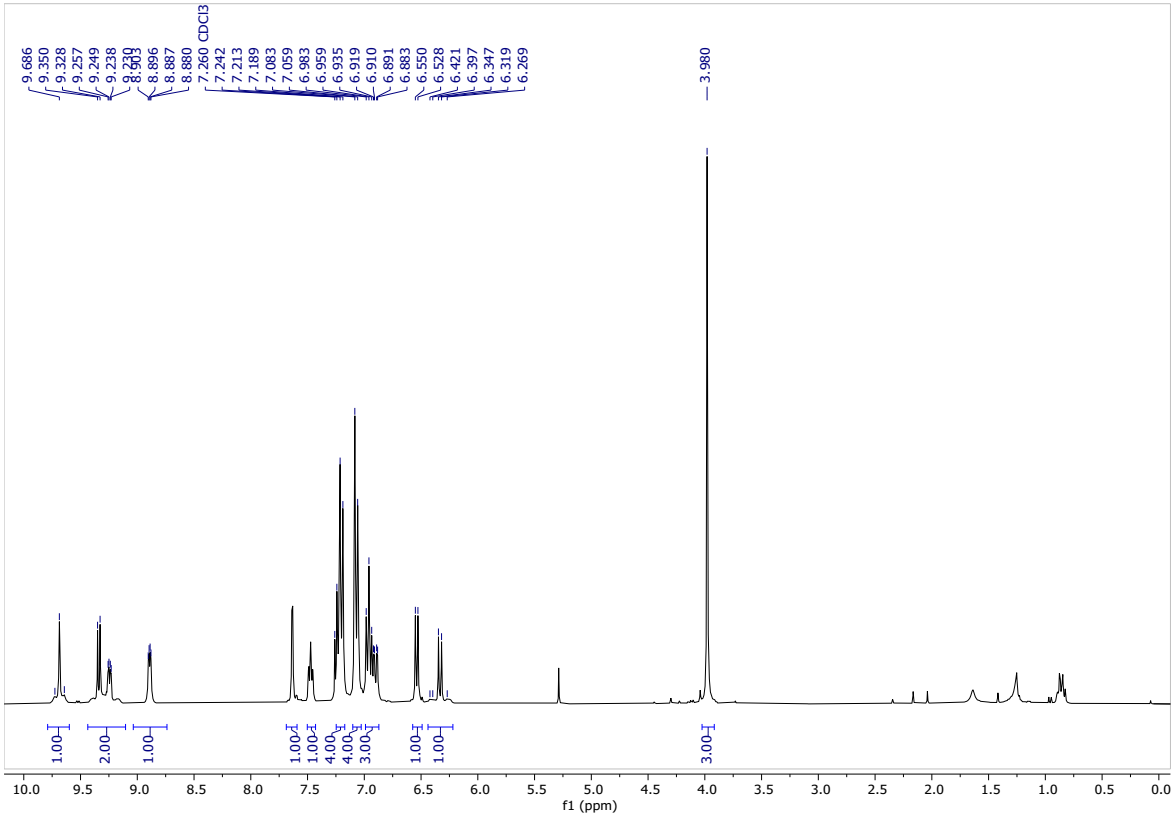


Fig. S33. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **10**.

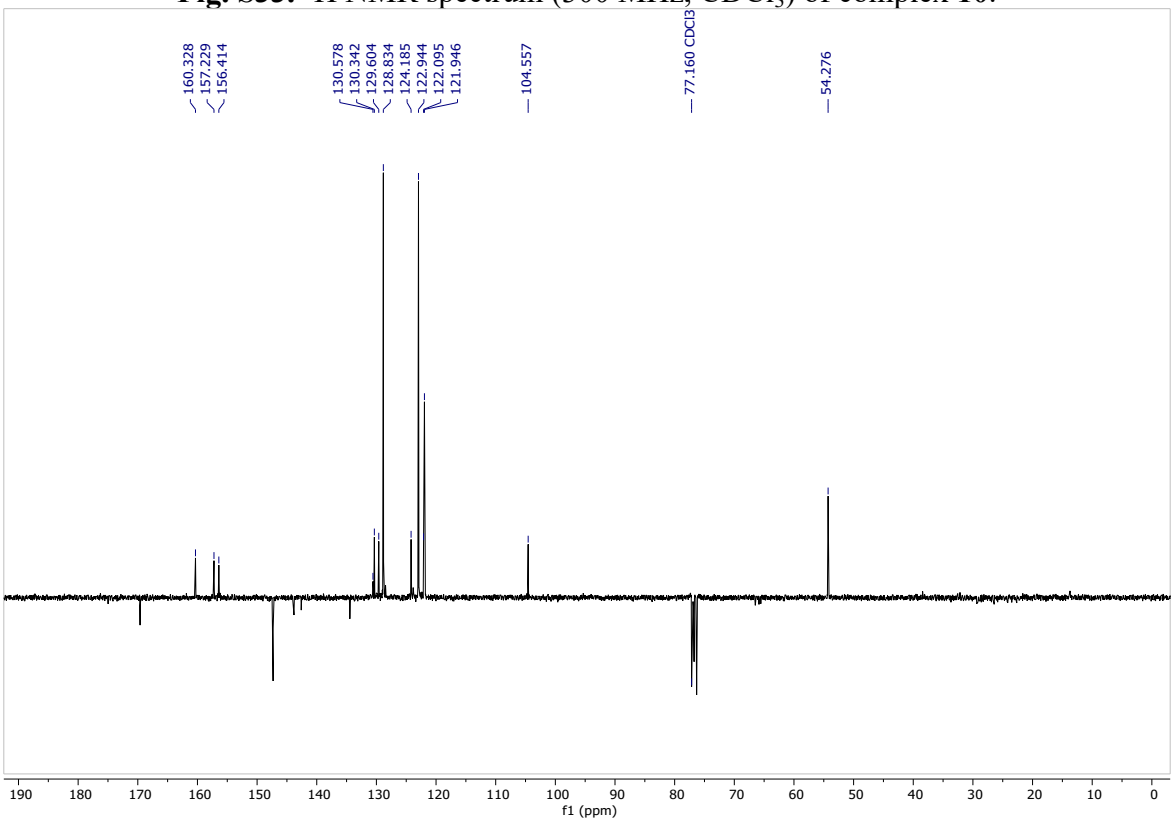


Fig. S34. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **10**.

Complex **11**

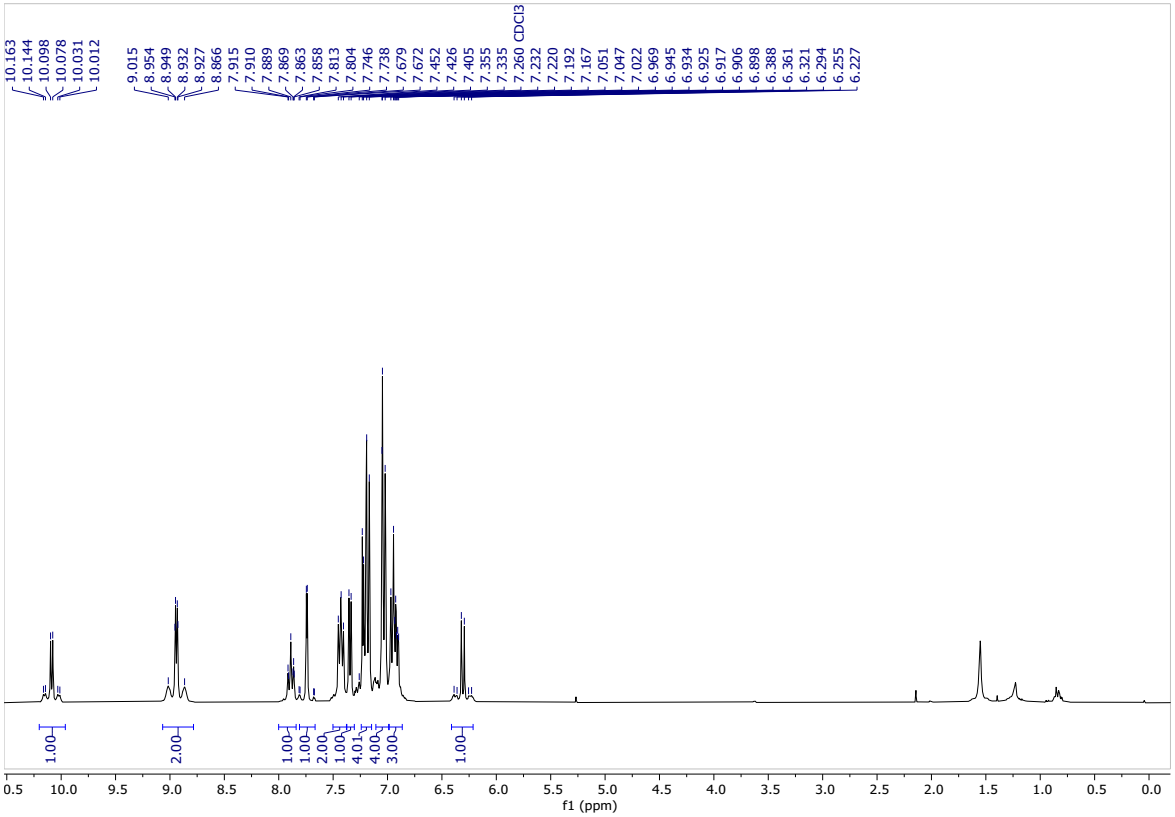


Fig. S35. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **11**.

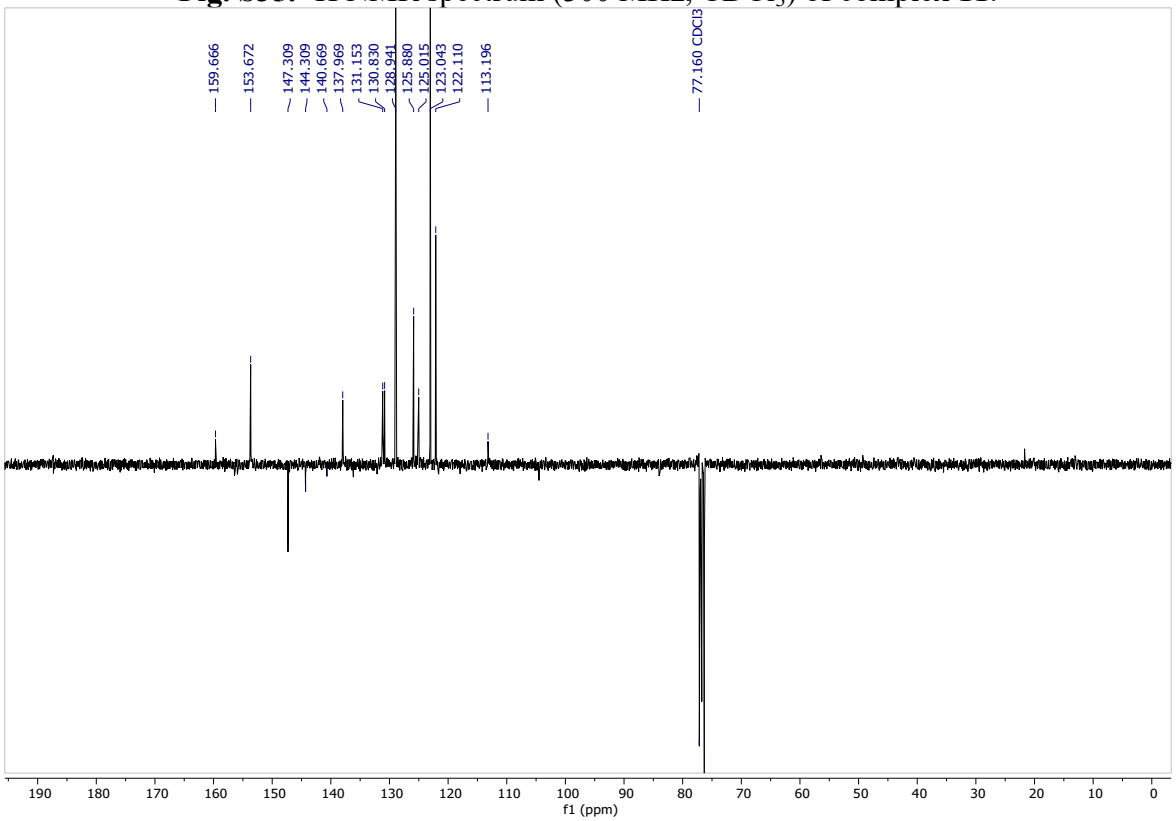


Fig. S36. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **11**.

Complex **12**

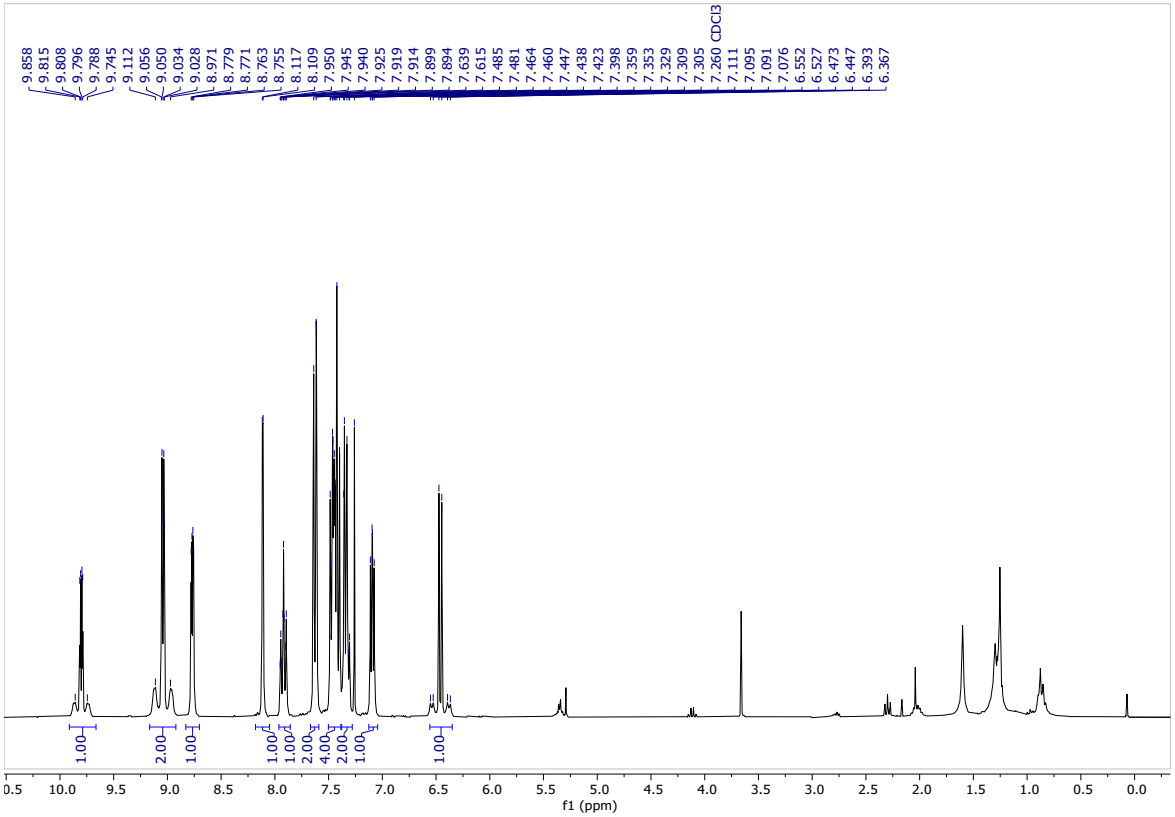


Fig. S37. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **12**.

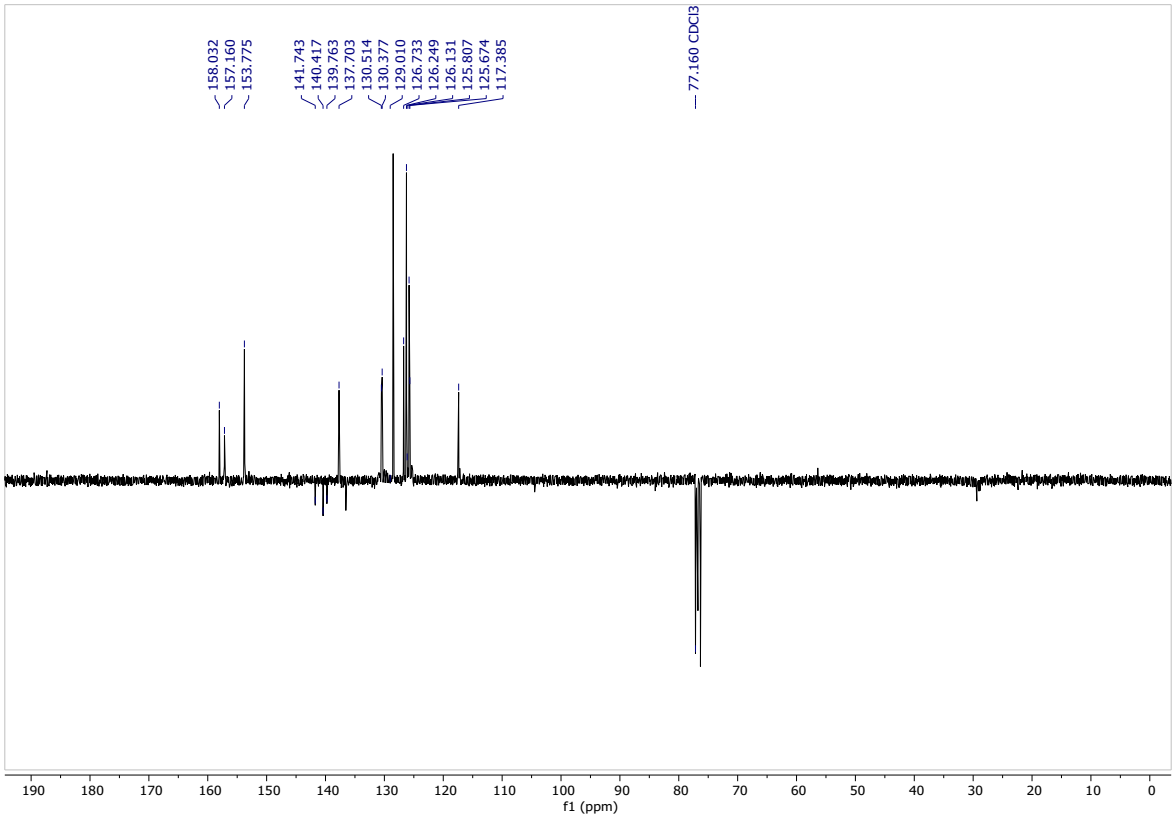


Fig. S38. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **12**.

Complex **13**

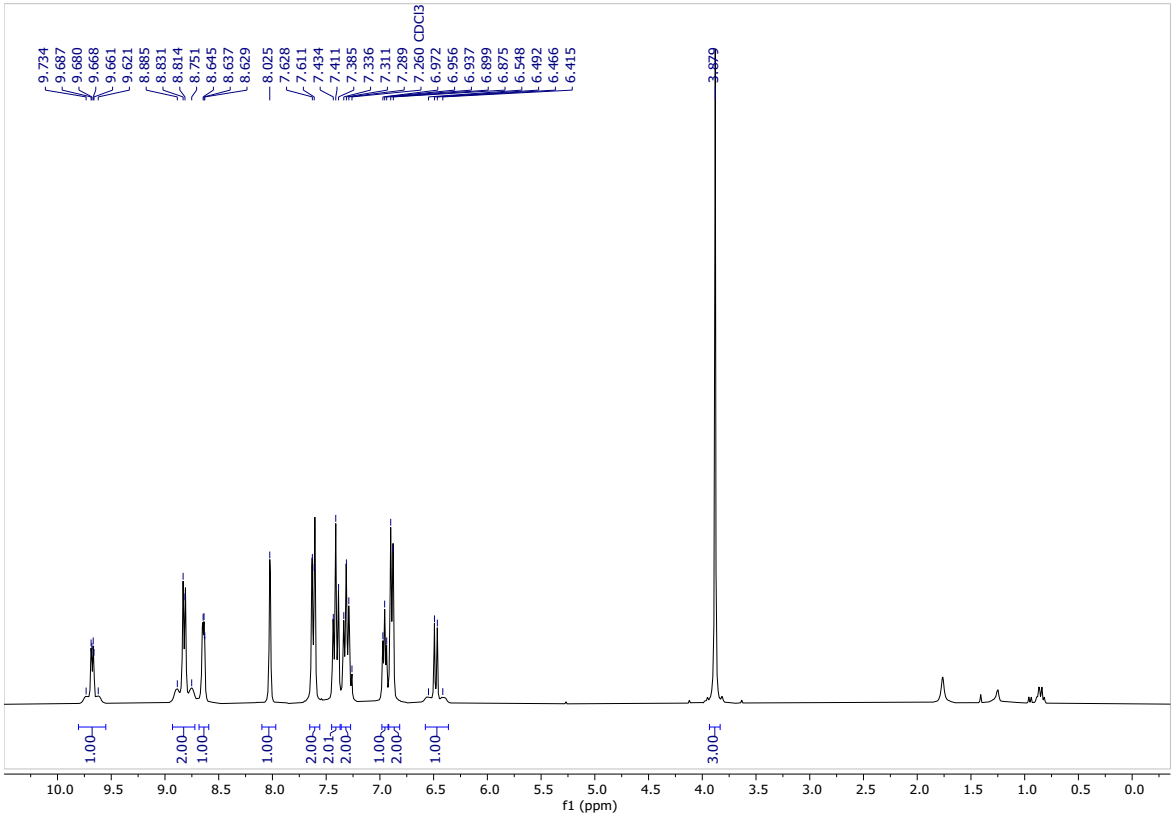


Fig. S39. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **13**.

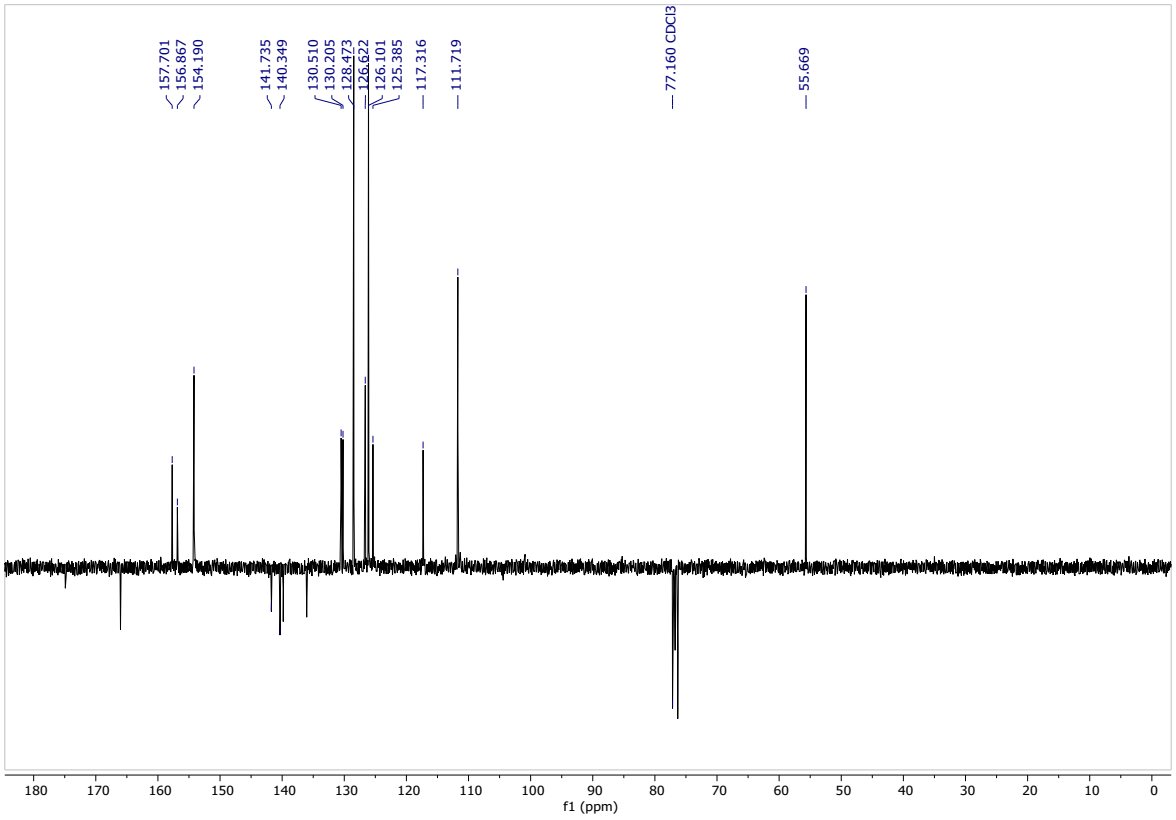


Fig. S40. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **13**.

Complex **14**

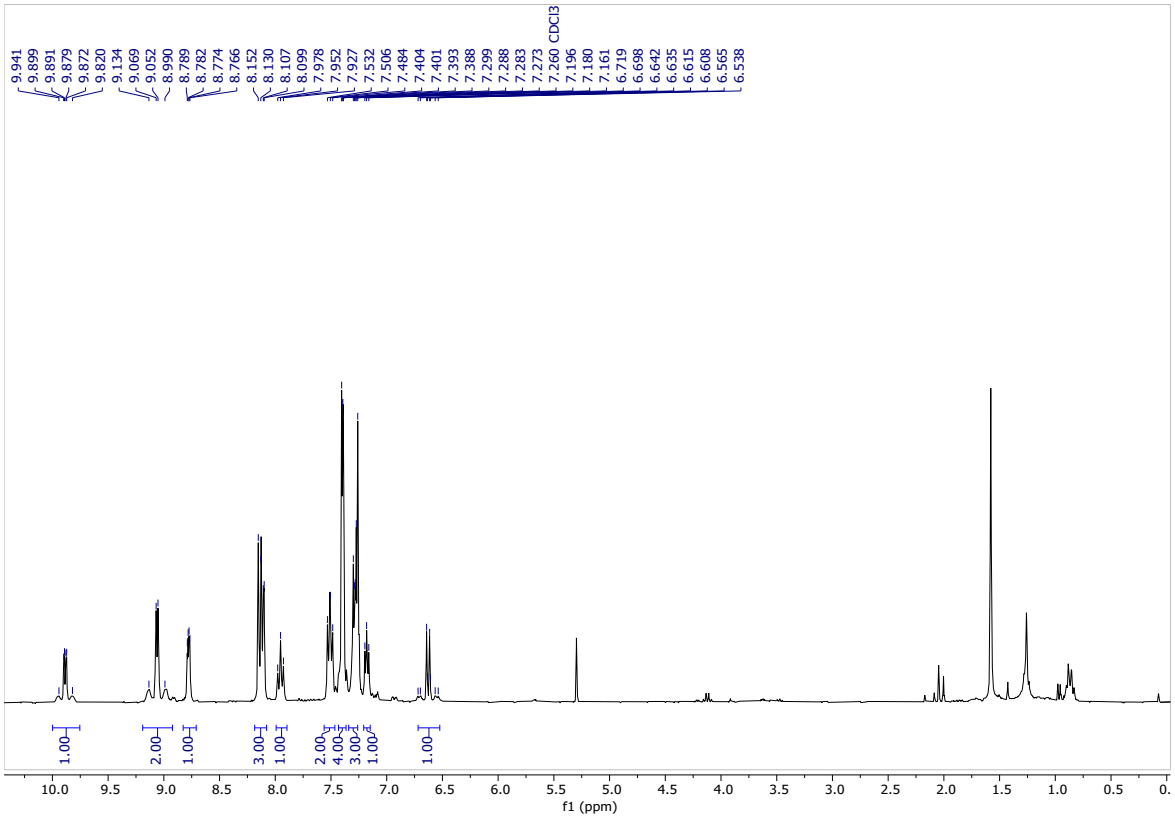


Fig. S41. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **14**.

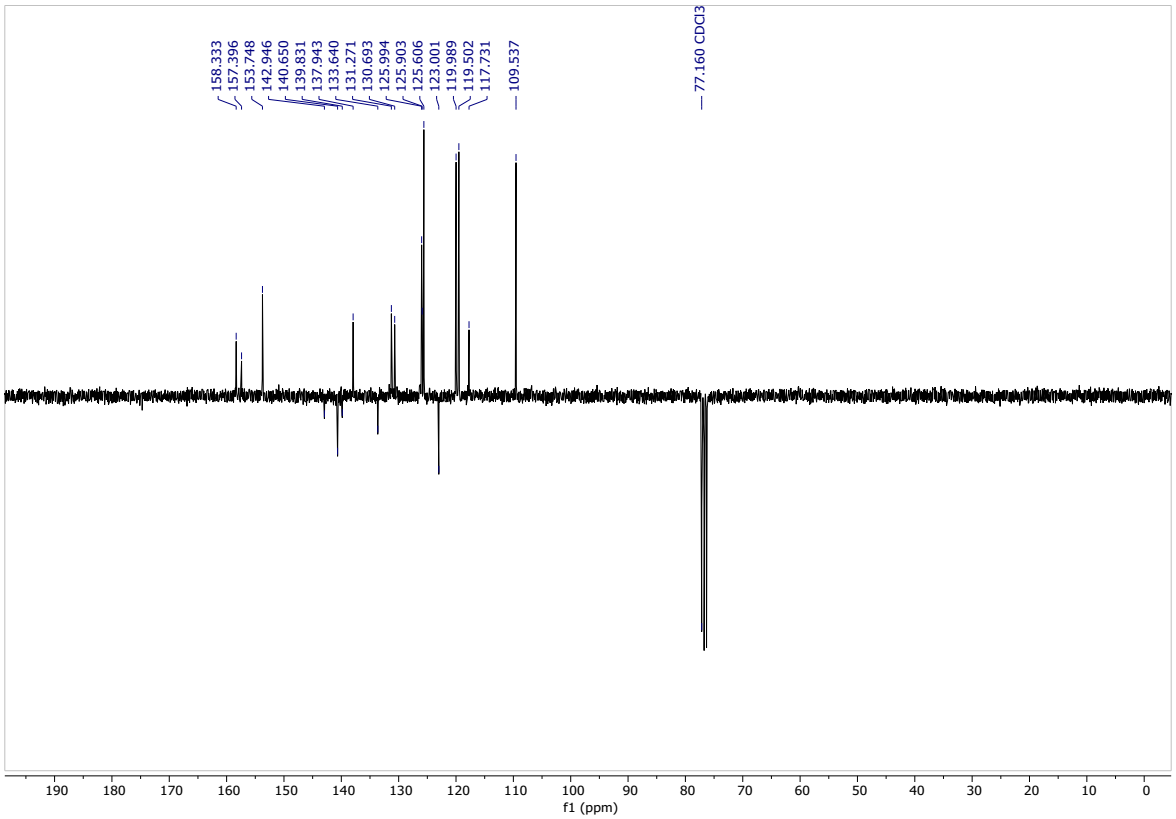


Fig. S42. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **14**.

Complex **15**

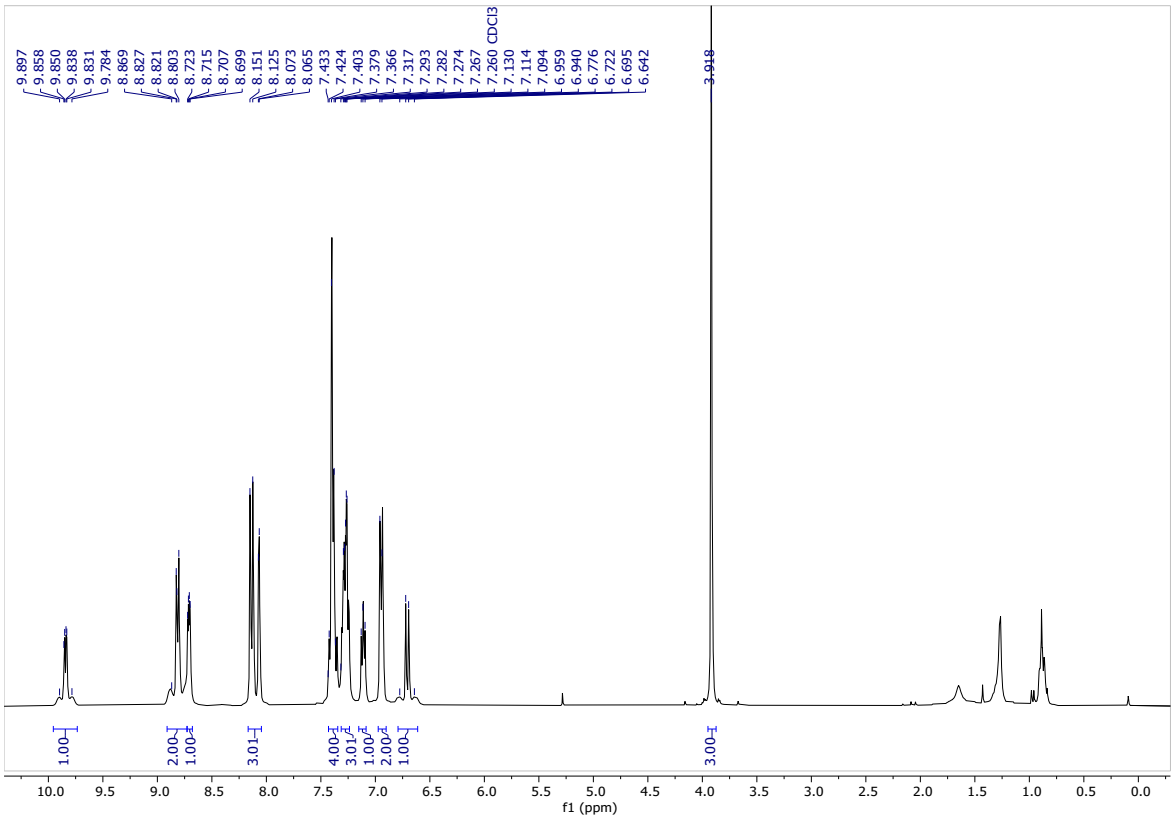


Fig. S43. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **15**.

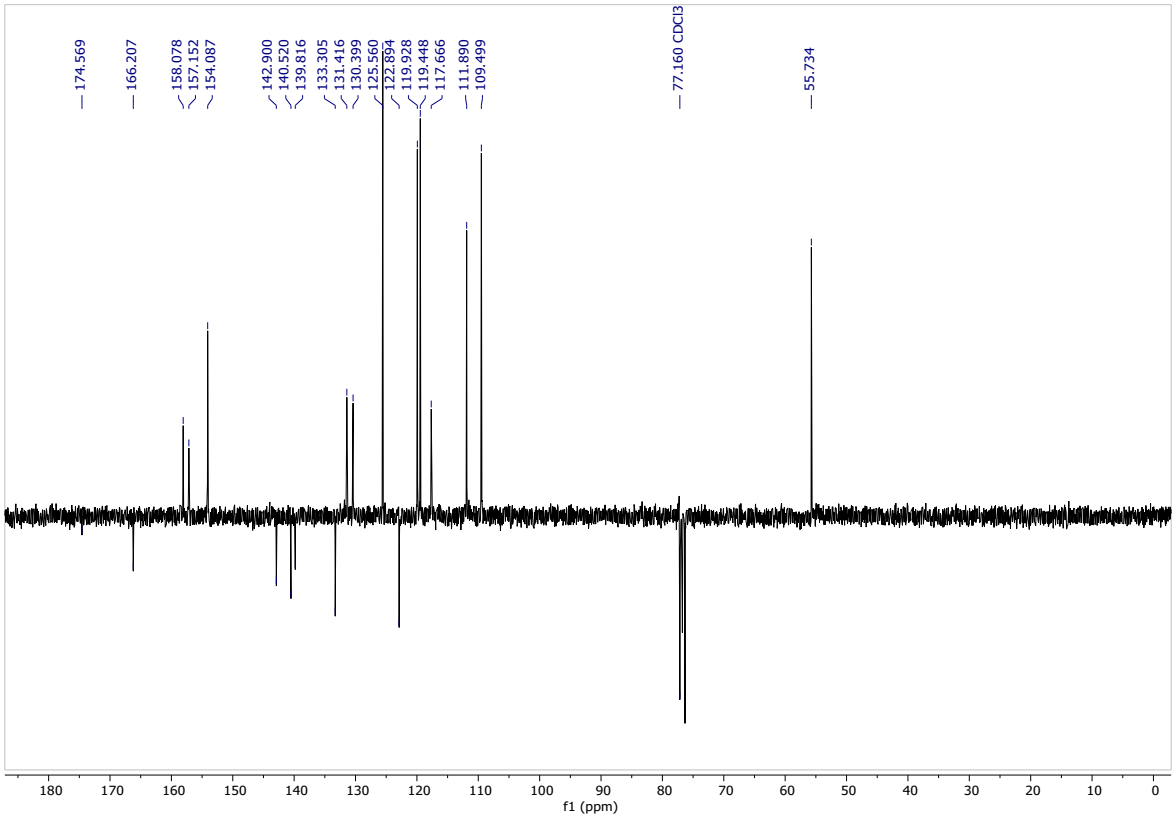


Fig. S44. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **15**.

Complex **16**

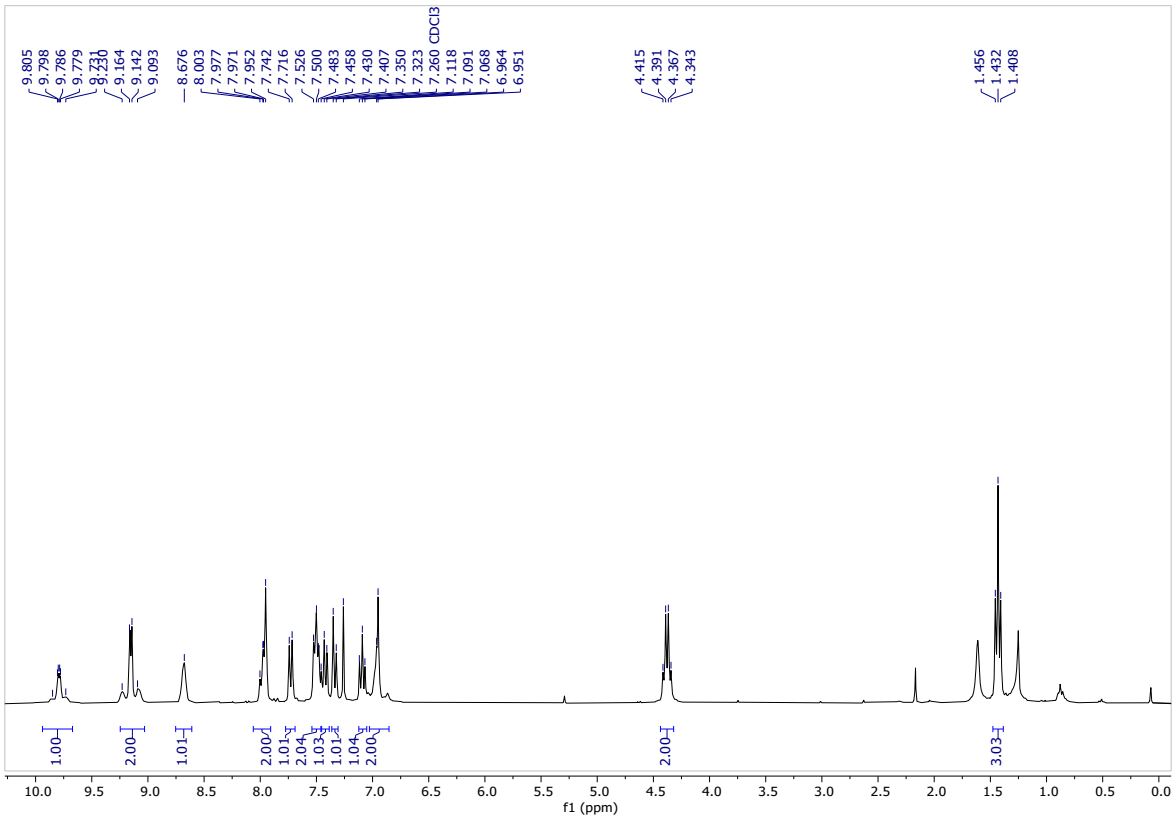


Fig. S45. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **16**.

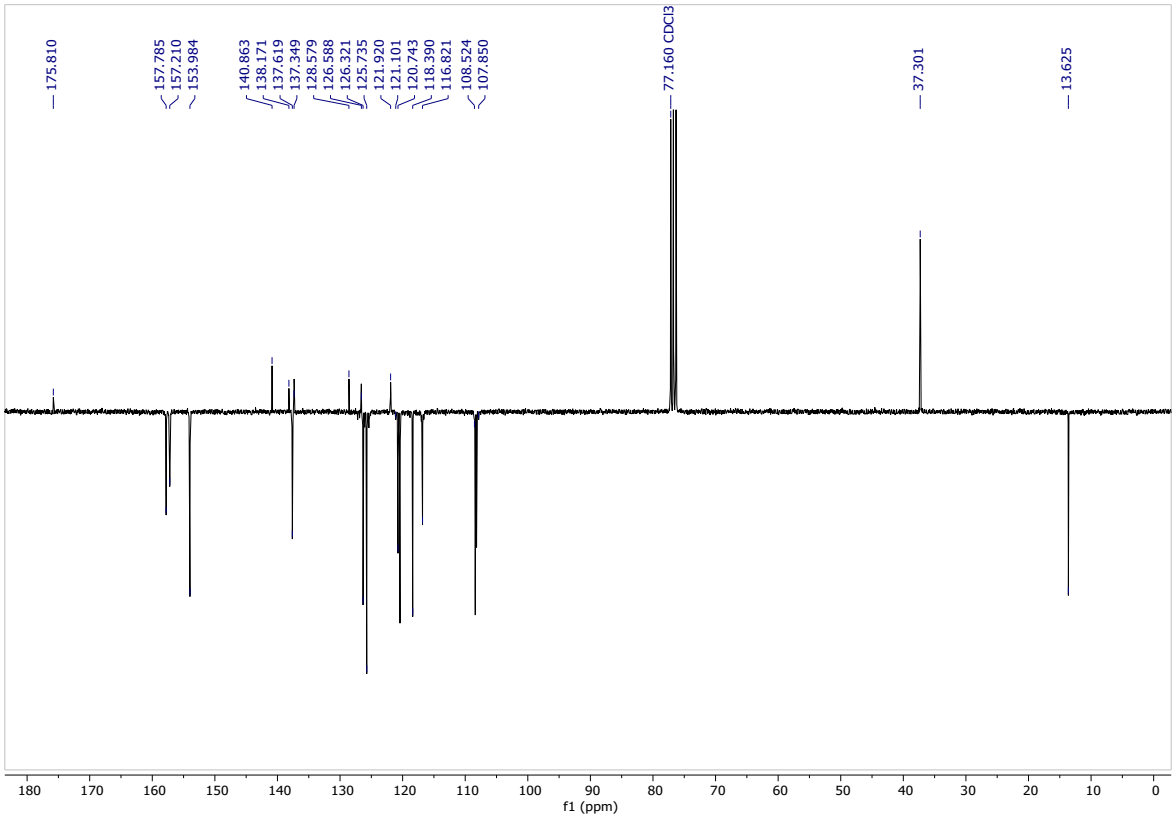


Fig. S46. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **16**.

Complex **17**

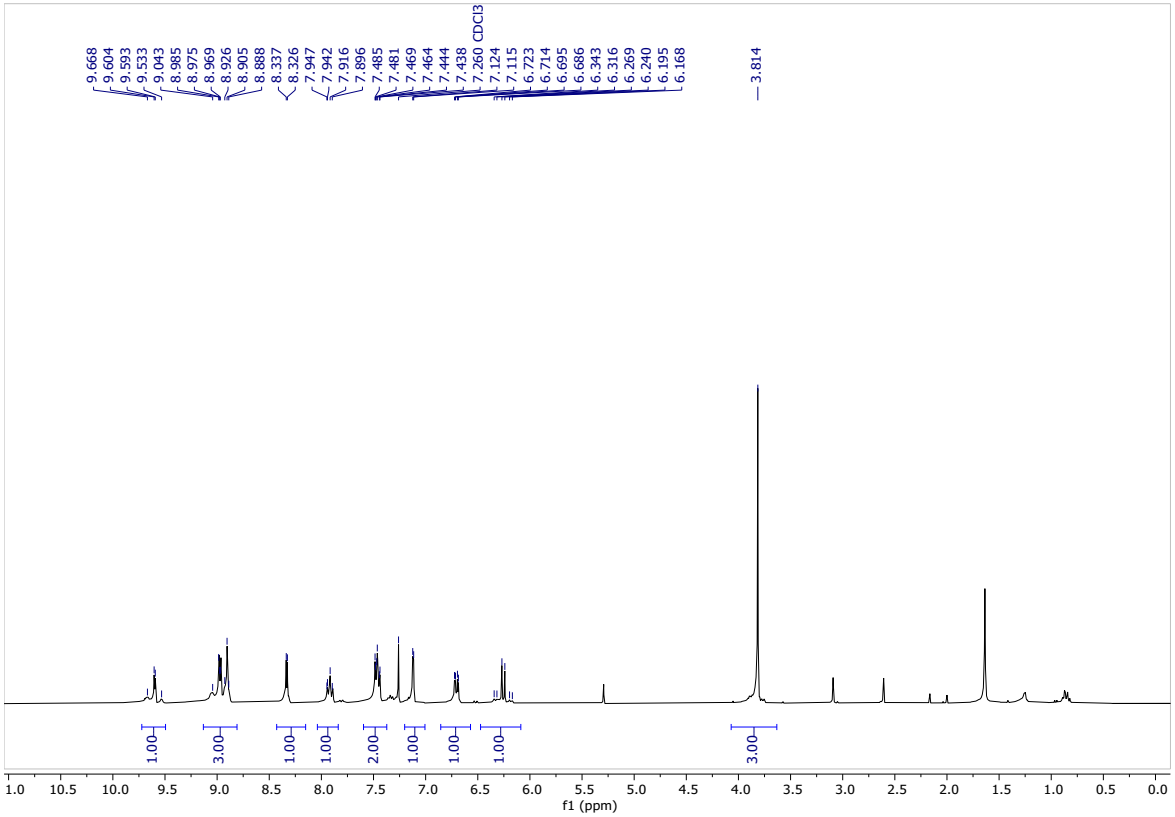


Fig. S47. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **17**.

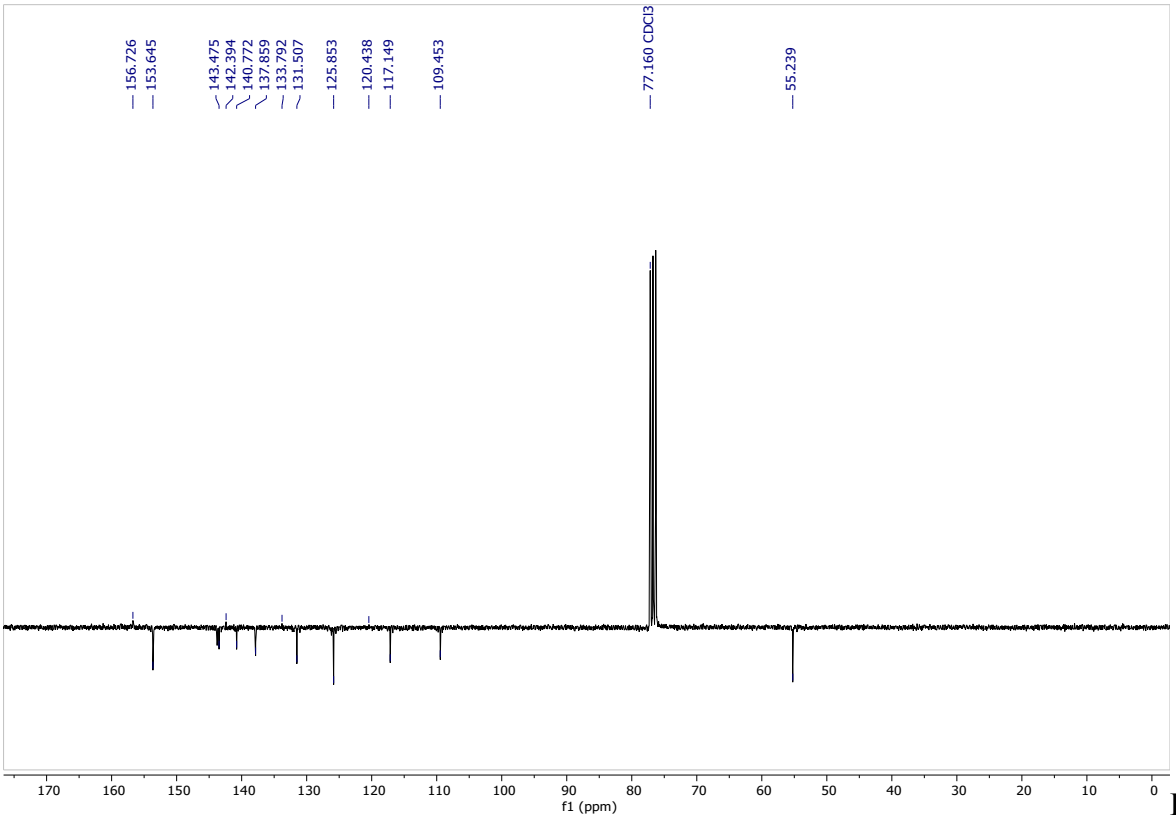


Fig. S48. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **17**.

Complex **18**

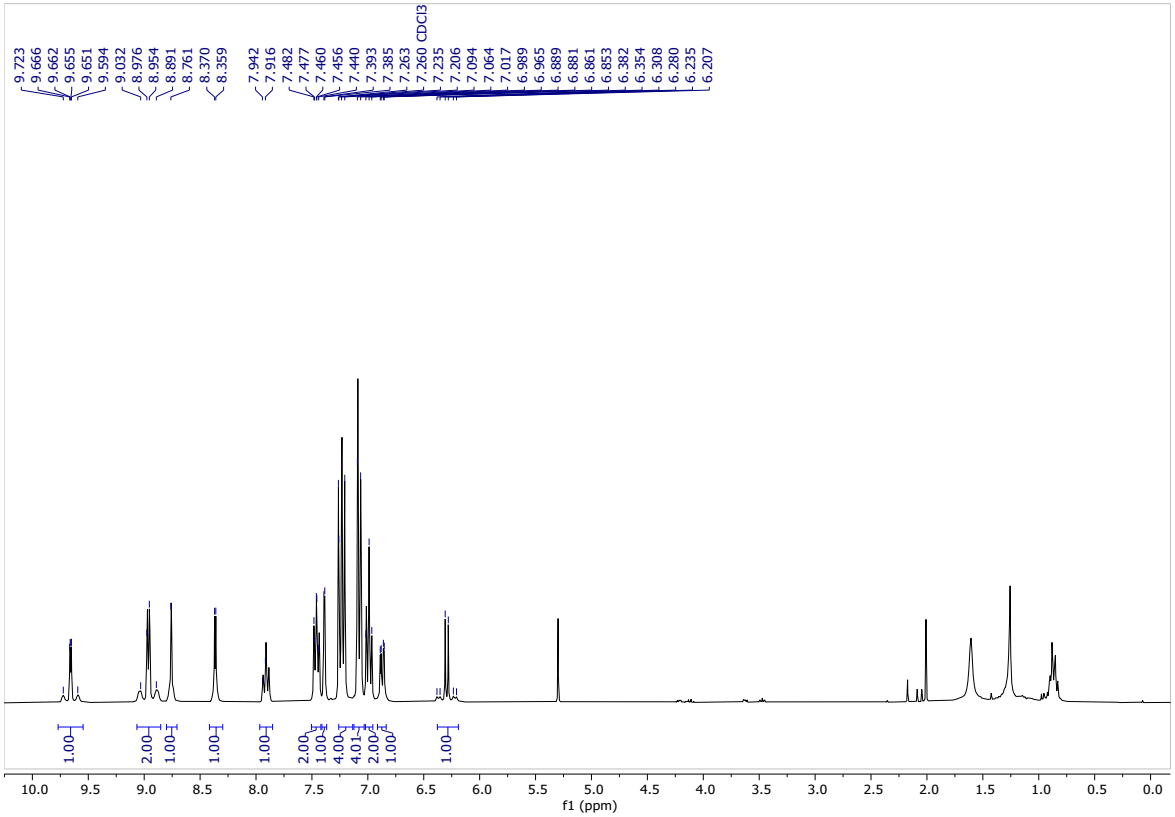


Fig. S49. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **18**.

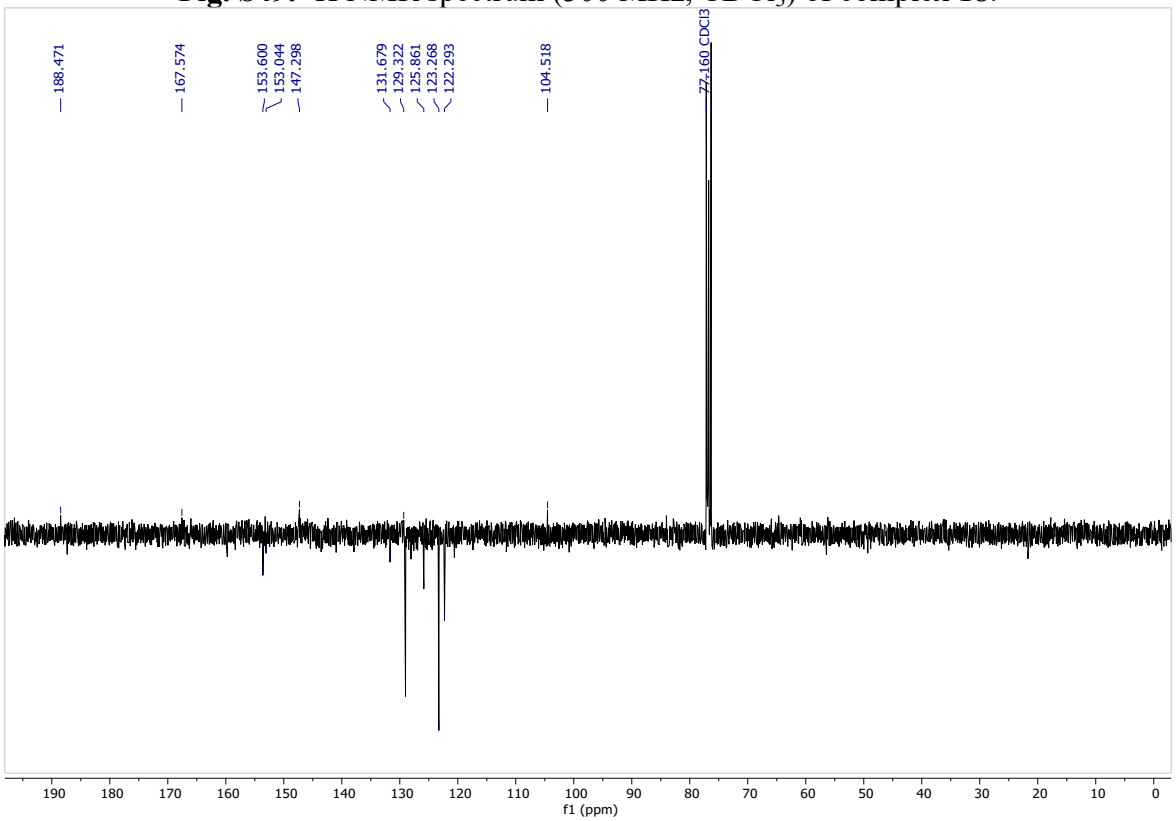


Fig. S50. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **18.**

Complex **19**

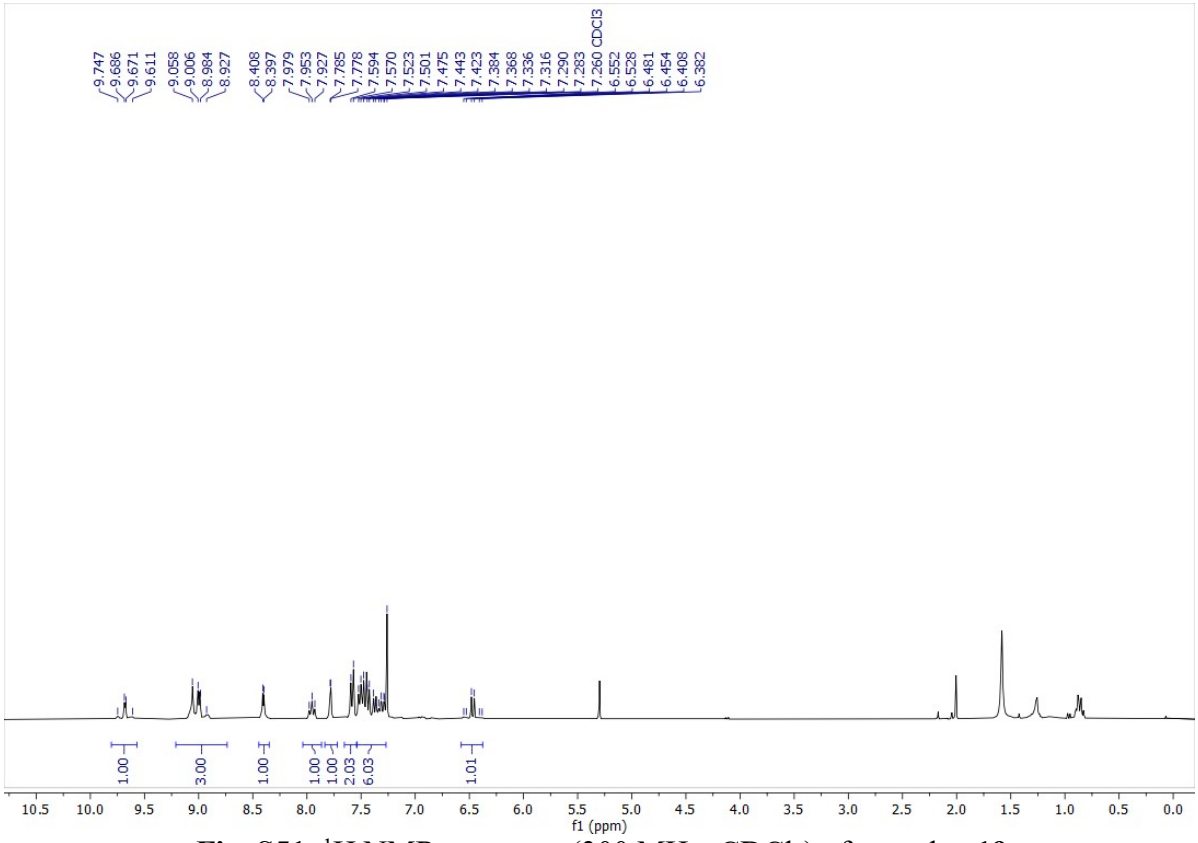


Fig. S51. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **19**.

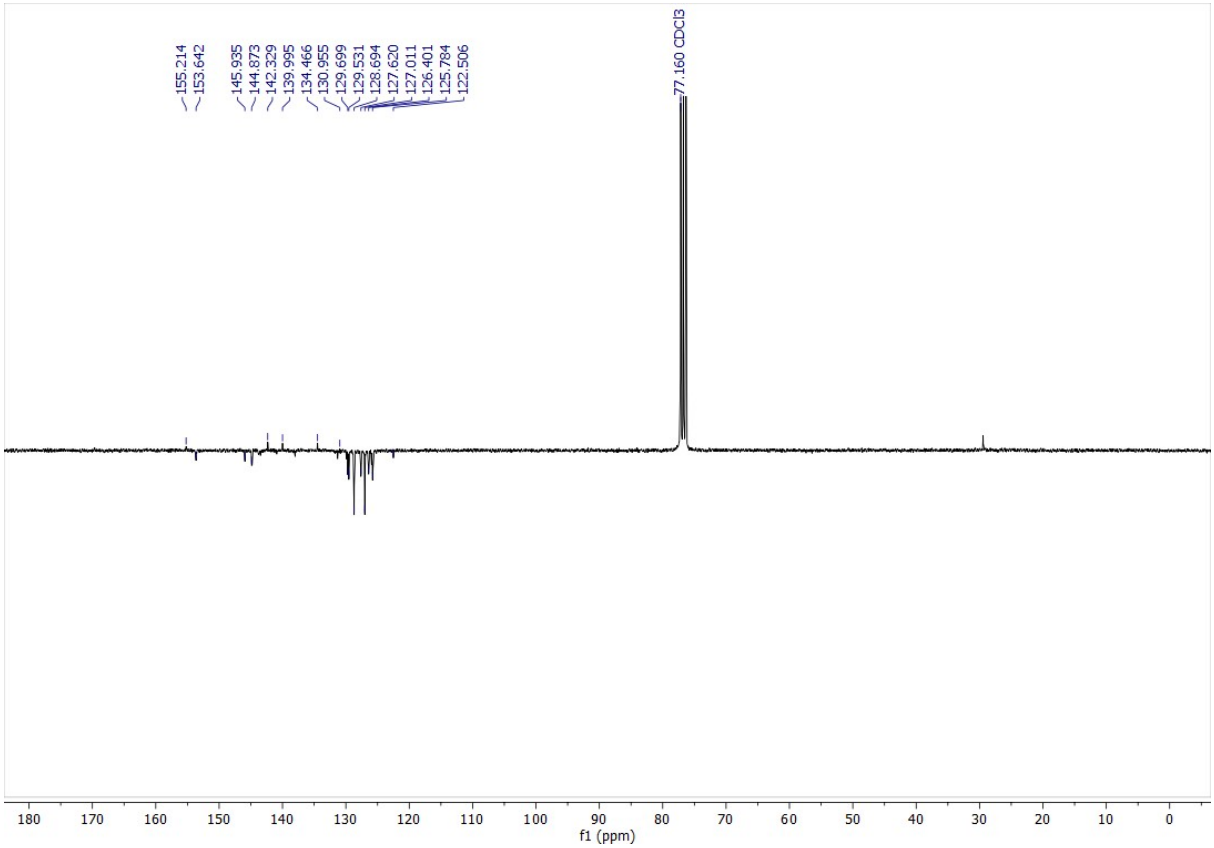


Fig. S52. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **19.**

Complex **20**

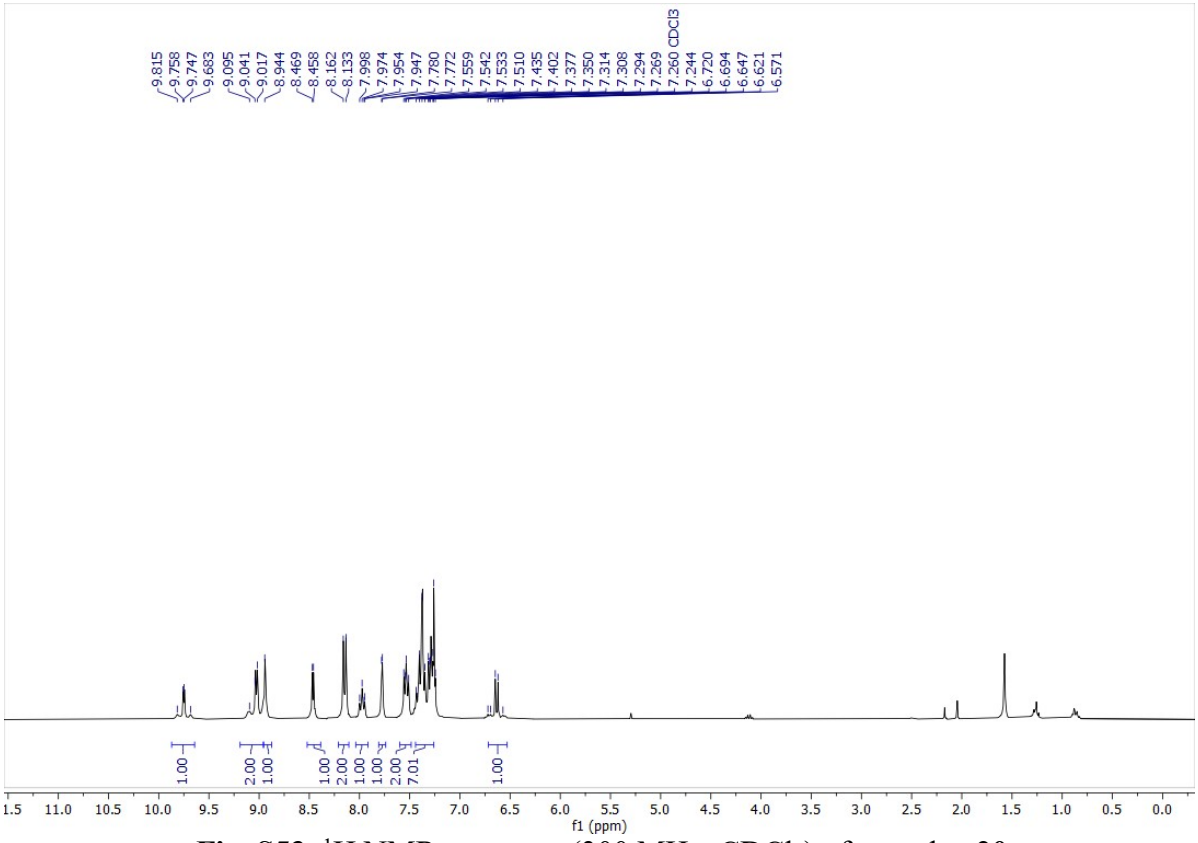


Fig. S53. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **20**.

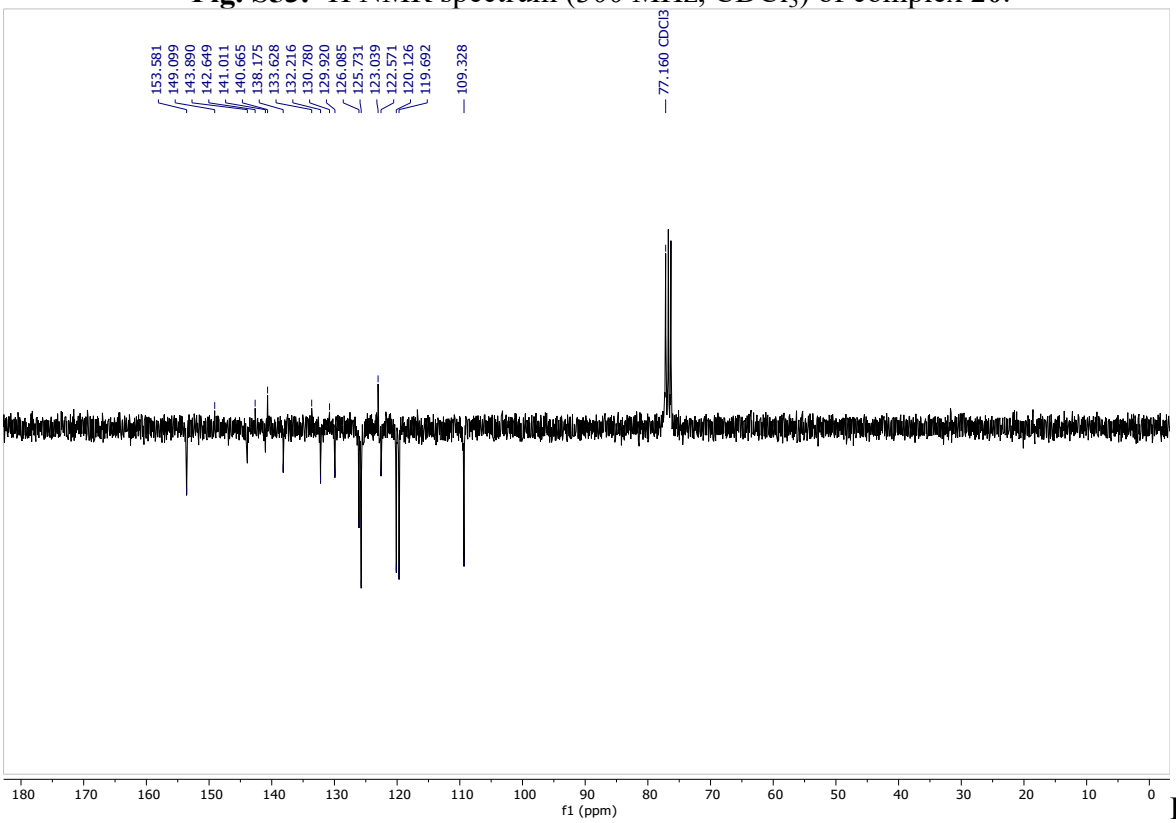


Fig. S54. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **20**.

Complex **21**

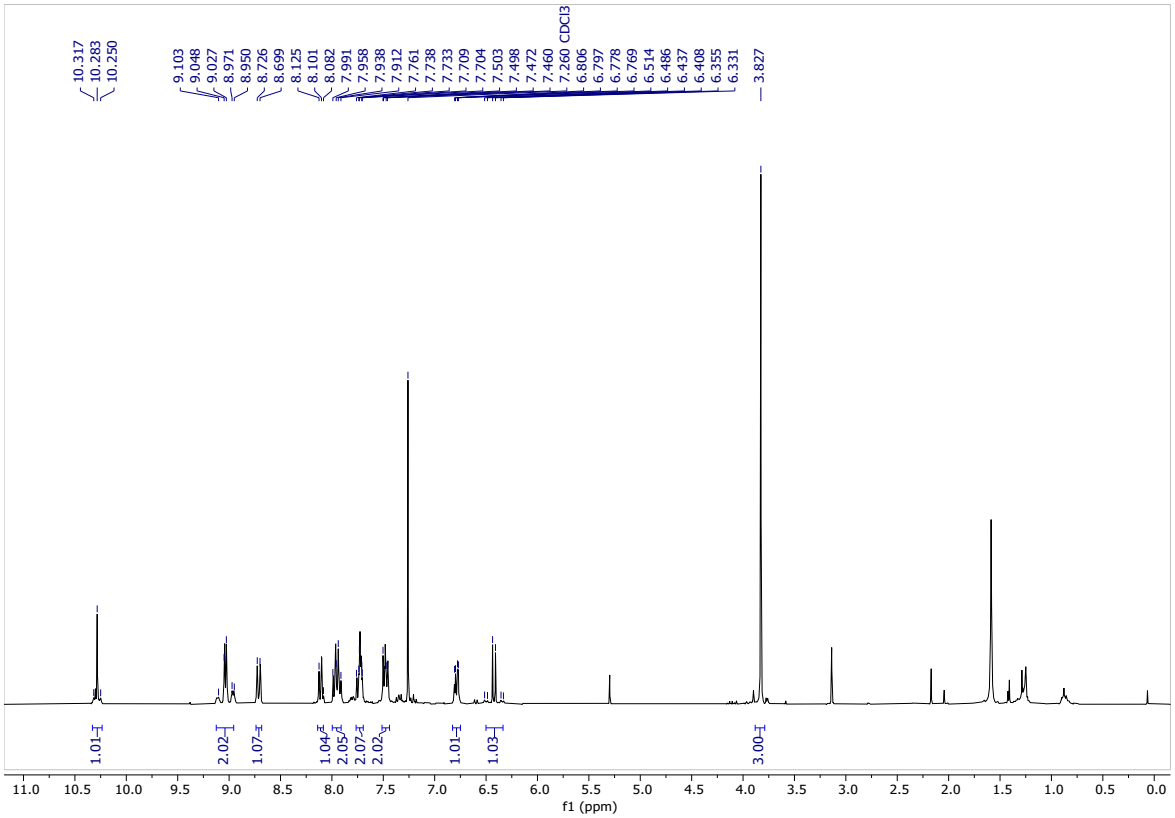


Fig. S55. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **21**.

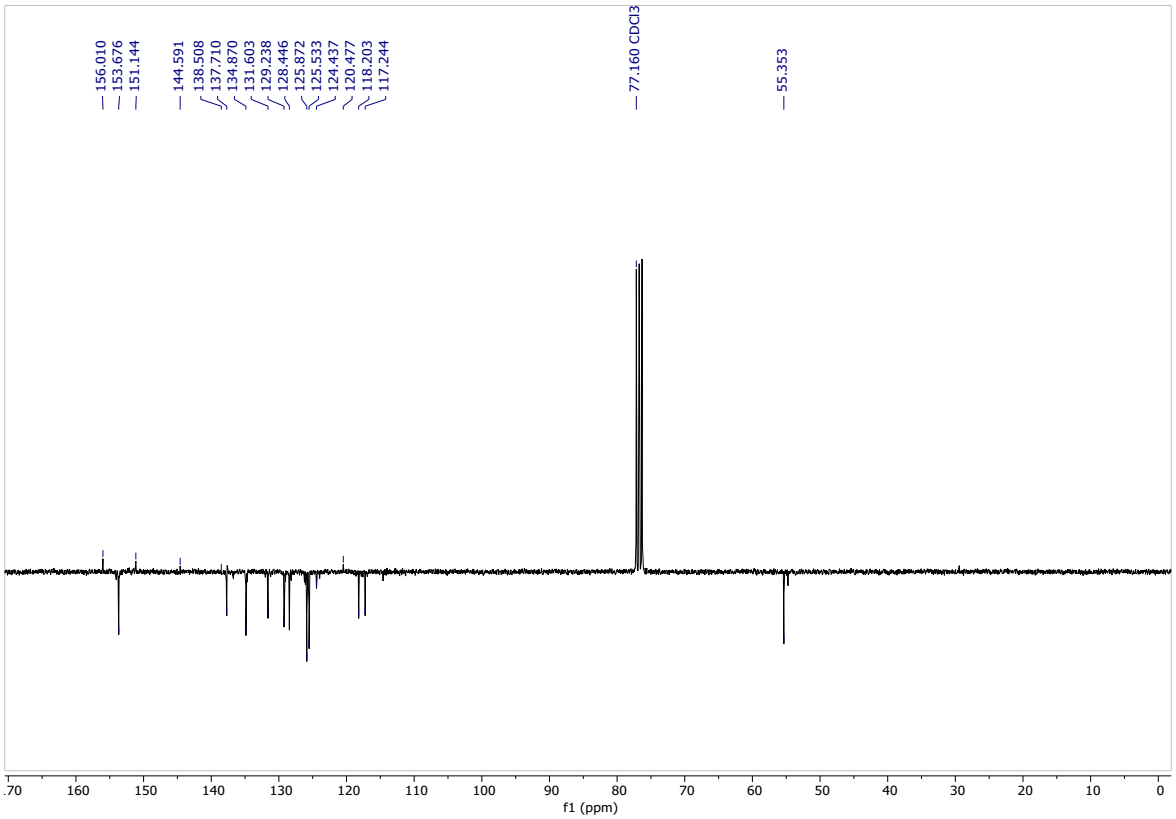


Fig. S56. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **21**.

Complex **22**

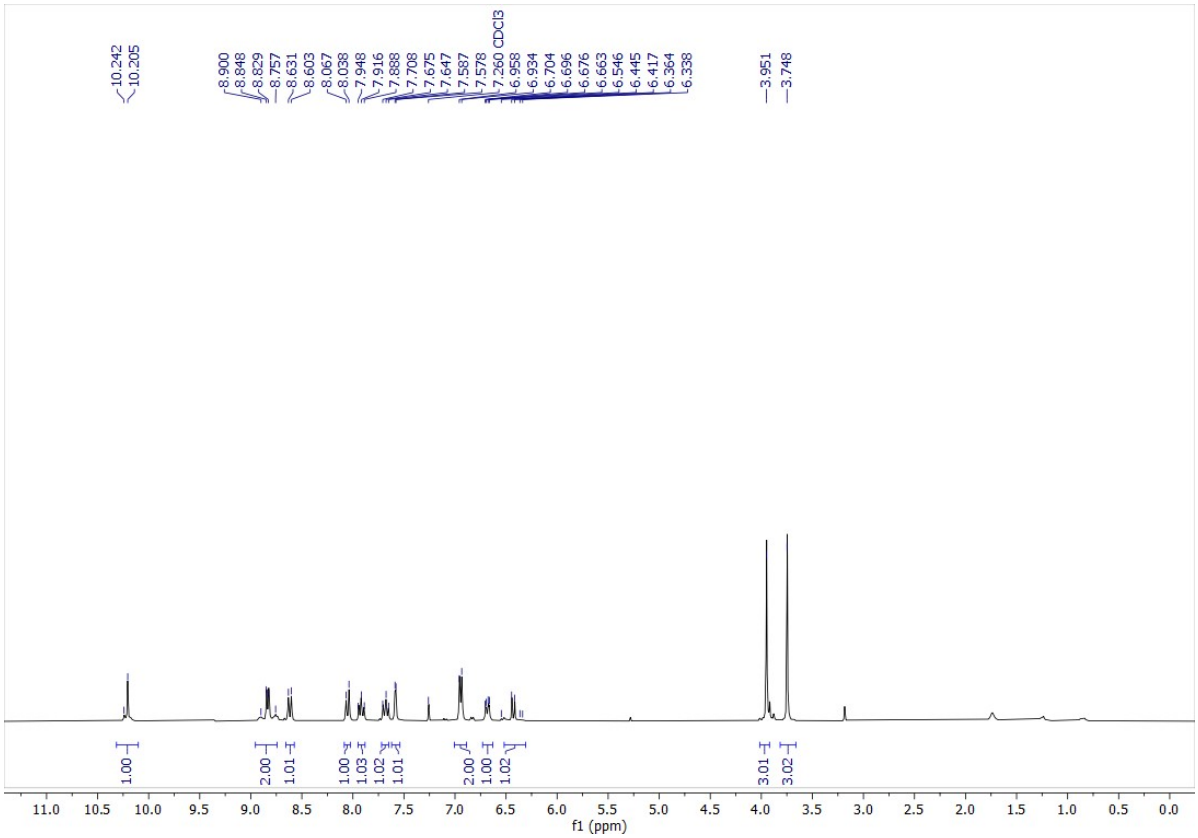


Fig. S57. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **22**.

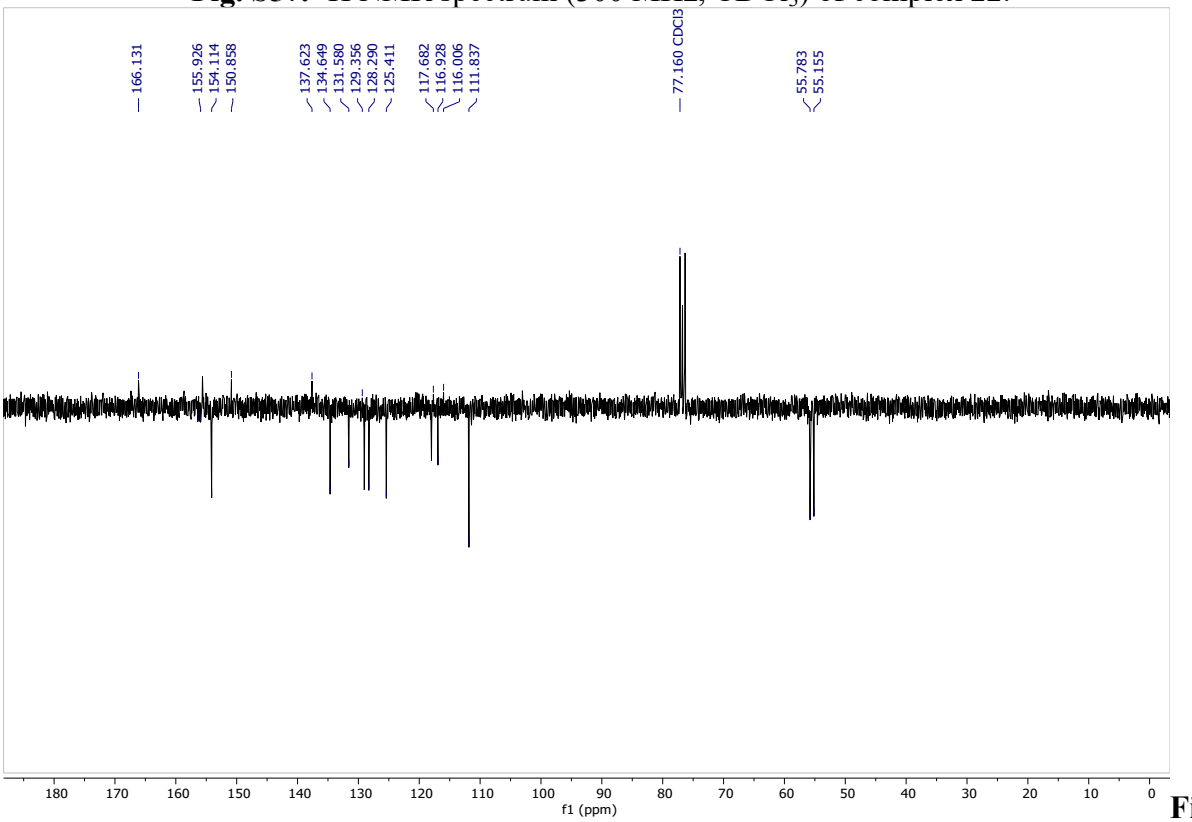


Fig. S58. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **22**.

Complex **23**

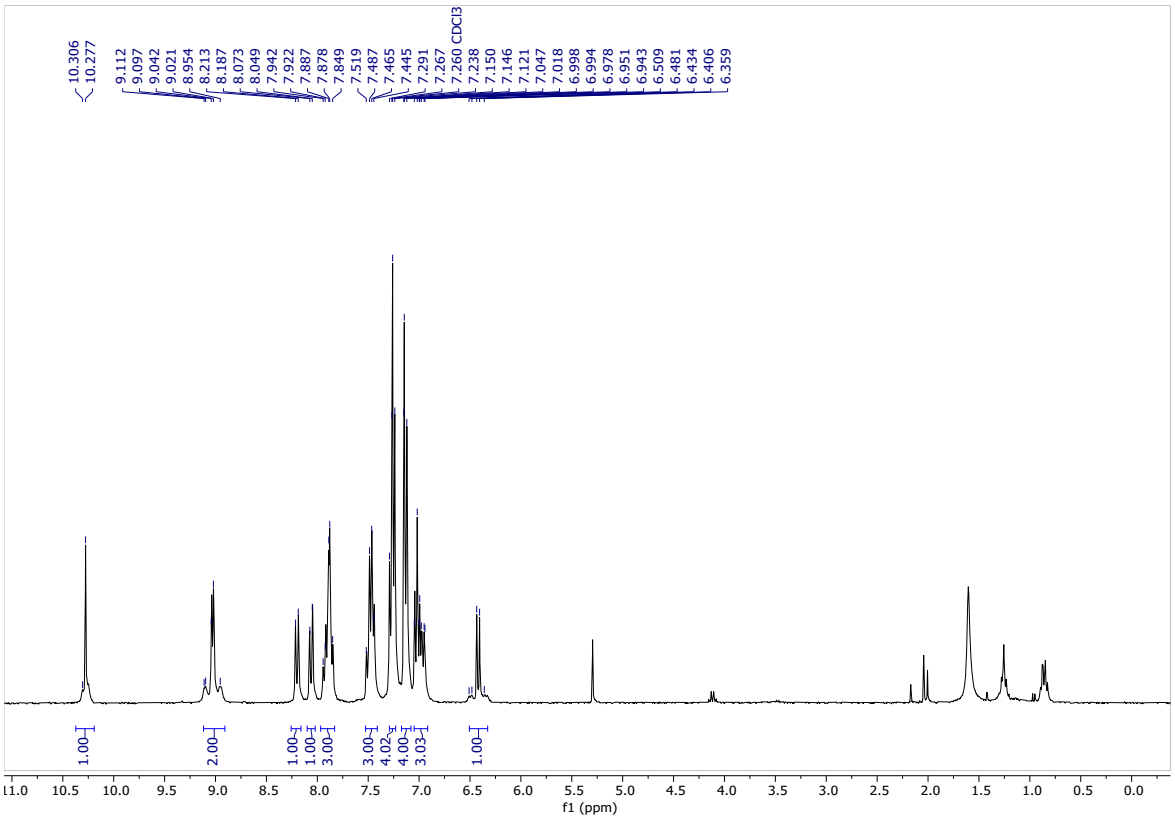


Fig. S59. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **23**.

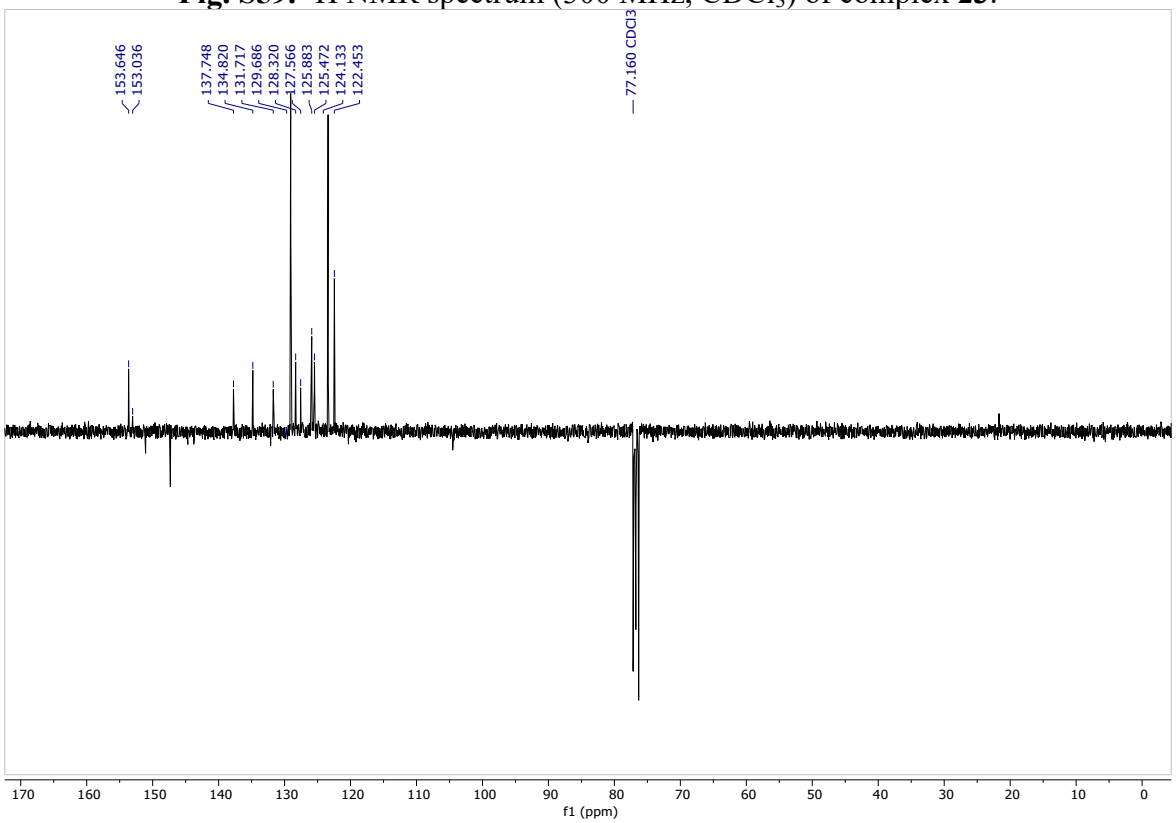


Fig. S60. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **23**.

Complex **24**

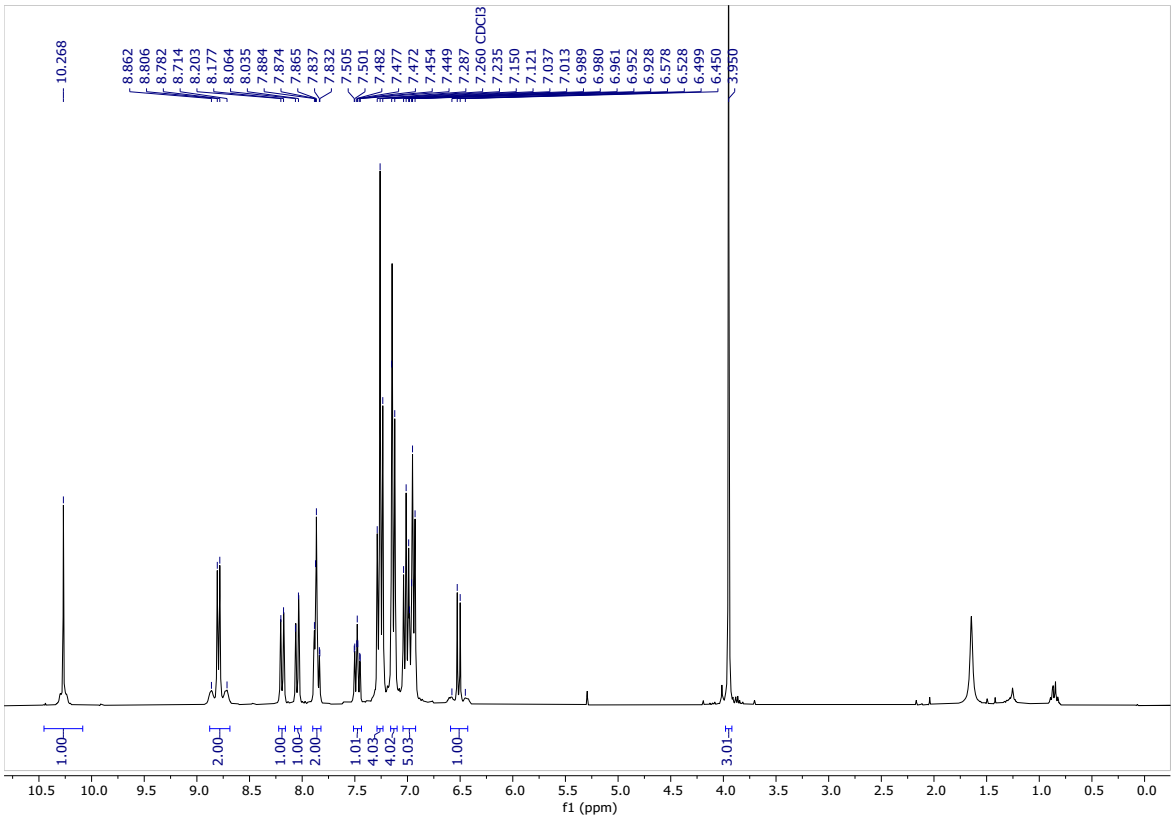


Fig. S61. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of complex **24**.

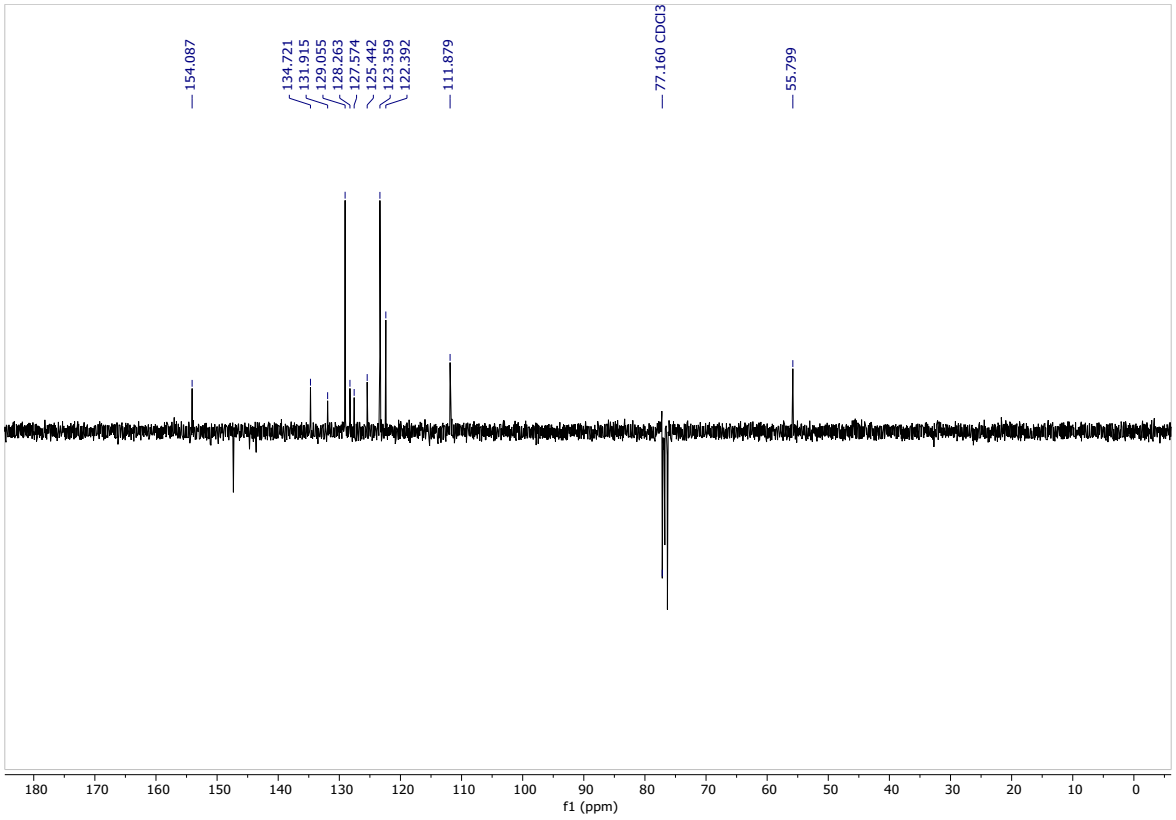


Fig. S62. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of complex **24**.

Crystallographic Data

Table S1 Crystallographic data for **7** + hexane (C_6H_{14})

Complex 7: crystal Data for C_{28} H_{23} Cl N_4 O Pt, (M = 662.05), triclinic, space group P-1, a = 9.0087(9), b = 10.5776(12), c = 17.4264(19) Å, α = 98,163(5), β = 104.652(4), γ = 101.634(5) °, V = 1540.6(3) $Å^3$. Z = 2, d = 1.613 $g.cm^{-3}$, μ = 4.674 mm^{-1}. The structure was solved by dual-space algorithm using the SHELXT program,[12] and then refined with full-matrix least-square methods based on F^2 (SHELXL).[13] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 6996 unique intensities and 360 parameters converged at ω$R(F^2)$ = 0.0852 (R(F) = 0.0424) for 6467 observed reflections with I > 2σ(I).

Crystallographic data for **7** + hexane (C_6H_{14})

Compound	**7**	
Empirical formula	C34 H37 Cl N4 O Pt	
CCDC	2211426	
Formula weight	748.21	
Temperature	150 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.0087(9) Å	a= 98.163(5)°.
	b = 10.5776(12) Å	b= 104.652(4)°.
	c = 17.4264(19) Å	g = 101.634(5)°.
Volume	1540.6(3) $Å^3$	
Z	2	
Density (calculated)	1.613 g/cm^3	
Absorption coefficient	4.674 mm^{-1}	
F(000)	744	
Crystal size	0.480 x 0.420 x 0.130 mm	
Crystal color	orange	
Theta range for data collection	2.132 to 27.475°.	
Index ranges	-11<=h<=11, -13<=k<=13, -22<=l<=22	
Reflections collected	20079	
Independent reflections	6996 [R(int) = 0.0472]	
Reflections [I>2sigma(I)]	6467	
Completeness to theta max	98.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.545 and 0.269	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6996 / 19 / 360	
Goodness-of-fit on F^2	1.102	
Final R indices [I>2sigma(I)]	R_1 = 0.0299, wR_2 = 0.0742	
R indices (all data)	R_1 = 0.0328, wR_2 = 0.0753	
Largest diff. peak and hole	1.873 and -0.993 e.$Å^{-3}$	

Table S2 Crystallographic data for **12**

Complex 12: crystal Data for C_{21} H_{16} Cl N_3 Pt, (*M* = 540.91), monoclinic, space group P 21/c (I.T.#14*)*, a = 11.6802(10), b = 7.3821(7), c = 20.8746(18) Å, α = 90°, β = 94.571(3), γ = 90°, V = 1794.2(3) $Å^3$. Z = 4, d = 2.002 $g.cm^{-3}$, μ = 7.979 mm^{-1}. The structure was solved by dual-space algorithm using the SHELXT program,[12] and then refined with full-matrix least-square methods based on F^2 (SHELXL).[13] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 4075 unique intensities and 235 parameters converged at ω$R(F^2)$ = 0.0699 (R(F) = 0.0285) for 3545 observed reflections with I > 2σ(I).

Crystallographic data for **12**

Compound	**12**	
Empirical formula	C21 H16 Cl N3 Pt	
CCDC	2211427	
Formula weight	540.91	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c (I.T.#14*)*	
Unit cell dimensions	a = 11.6802(10)Å	a= 90°.
	b = 7.3821(7) Å	b= 94.571(3)°.
	c = 20.8746(18) Å	g = 90°.
Volume	15794.2(3) $Å^3$	
Z	4	
Density (calculated)	2.002 g/cm^3	
Absorption coefficient	7.979 mm^{-1}	
F(000)	1032	
Crystal size	0.280 x 0.120 x 0.070 mm	
Crystal color	yellow	
Theta range for data collection	1.749 to 27.486°.	
Index ranges	-15<=h<=15, -9<=k<=9, -27<=l<=23	
Reflections collected	18884	
Independent reflections	4075 [R(int) = 0.0591]	
Reflections [I>2sigma(I)]	3545	
Completeness to theta max	98.8 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.572 and 0.338	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4075 / 0 / 235	
Goodness-of-fit on F^2	1.105	
Final R indices [I>2sigma(I)]	R_1 = 0.0285, wR_2 = 0.0699	
R indices (all data)	R_1 = 0.0337, wR_2 = 0.0733	
Largest diff. peak and hole	1.100 and -1.404 e.$Å^{-3}$	

Table S3: Crystallographic data for **14**+ 0.5 EtOAc

Complex 14: crystal Data for C_{27} H_{20} Cl N_4 Pt, (*M* = 5631.02), monoclinic, space group P 21/n, a = 12.4061(3), b = 7.9544(2), c = 25.2752(5) Å, α = 90°, β = 94.2180(10), γ = 90°, V = 1794.2(3) $Å^3$. Z = 4, d = 1.800 $g.cm^{-3}$, μ = 5.779 mm^{-1}. The structure was solved by dual-space algorithm using the SHELXT program,[12] and then refined with full-matrix least-square methods based on F^2 (SHELXL).[13] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 5683 unique intensities and 322 parameters converged at ω$R(F^2)$ = 0.0644 (R(F) = 0.0281) for 4968 observed reflections with I > 2σ(I).

Crystallographic data for **14** + 0.5 EtOAc

Compound	**14**	
Empirical formula	C29 H23 Cl N4 O Pt	
CCDC	2211428	
Formula weight	674.05	
Temperature	150 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic, P 21/n	
Space group	P 21/c (I.T.#14*)*	
Unit cell dimensions	a = 12.4061(3) Å	a= 90°.
	b = 7.9544(2) Å	b= 94.2180(10)°.
	c = 25.2752(5) Å	g = 90°.
Volume	2487.48(10) $Å^3$	
Z	4	
Density (calculated)	1.800 g/cm^3	
Absorption coefficient	5.779 mm^{-1}	
F(000)	1312	
Crystal size	0.340 x 0.220 x 0.200 mm	
Crystal color	yellow	
Theta range for data collection	2.685 to 27.477°.	
Index ranges	-16<=h<=15, -9<=k<=10, -32<=l<=32	
Reflections collected	19769	
Independent reflections	5683 [R(int) = 0.0421]	
Reflections [I>2sigma(I)]	4968	
Completeness to theta max	99.7 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.315 and 0.191	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5683 / 15 / 322	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R_1 = 0.0281, wR_2 = 0.0644	
R indices (all data)	R_1 = 0.0344, wR_2 = 0.0660	
Largest diff. peak and hole	1.808 and -1.323 $e.Å^{-3}$	

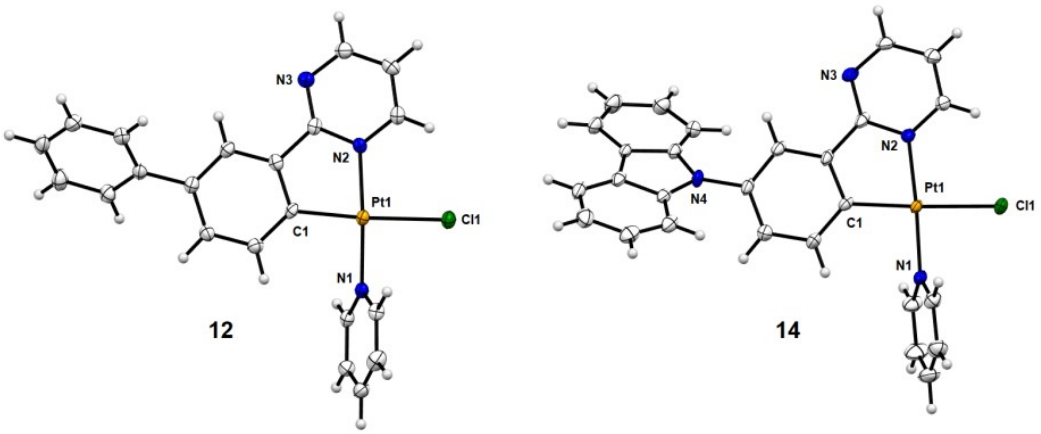


Fig. 63. ORTEP representation of complexes **12**, and **14** with 50% ellipsoid probability. All co-crystallized solvent molecules have been omitted for clarity.

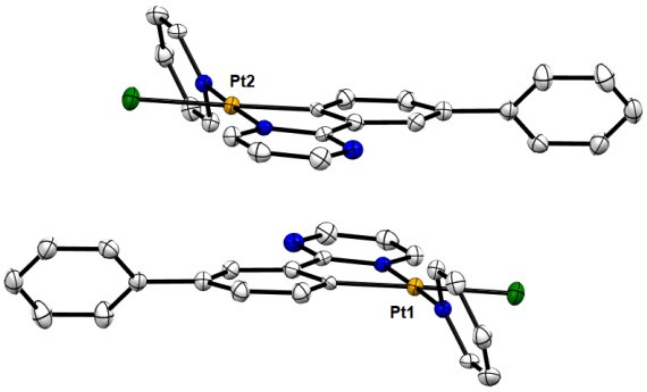


Fig. 64. ORTEP representation of the crystal packing structure in dimeric form: complex **12** showing the head-to-tail configuration. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms and all co-crystallized solvent molecules have been omitted for clarity.

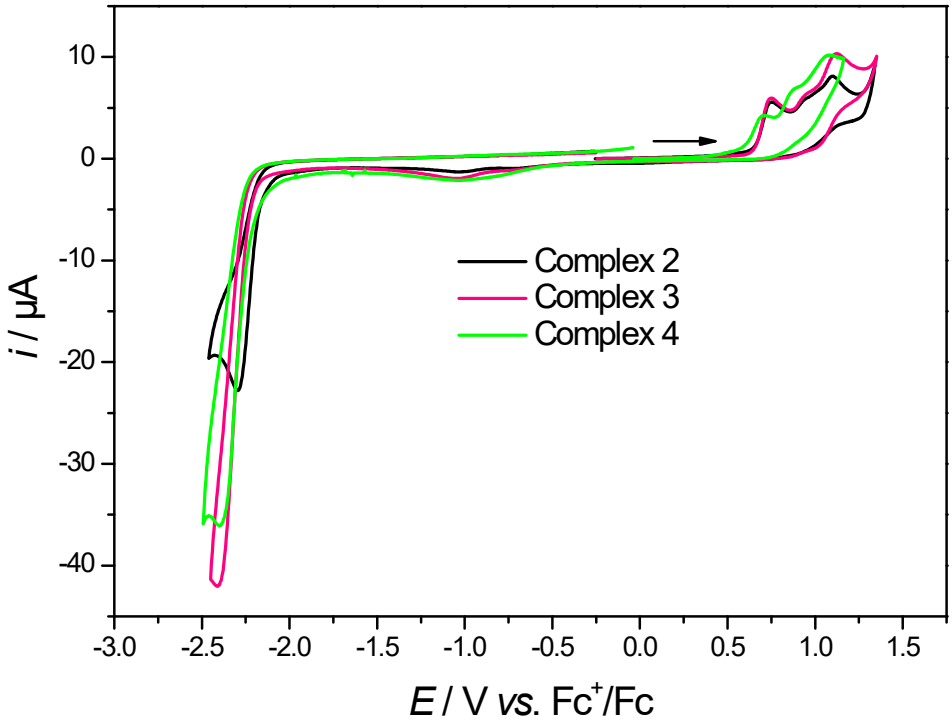


Fig. S65. Cyclic voltammograms of complexes **2** (black), **3** (red) and **4** (green) at a Pt working electrode in CH_2Cl_2/NBu_4PF_6 0.1 M (*E* / V *vs.* Fc^+/Fc, $v = 0.1$ V s^{-1}, $C = 0.5$ mM). The arrow indicates the scanning direction from the initial potential.

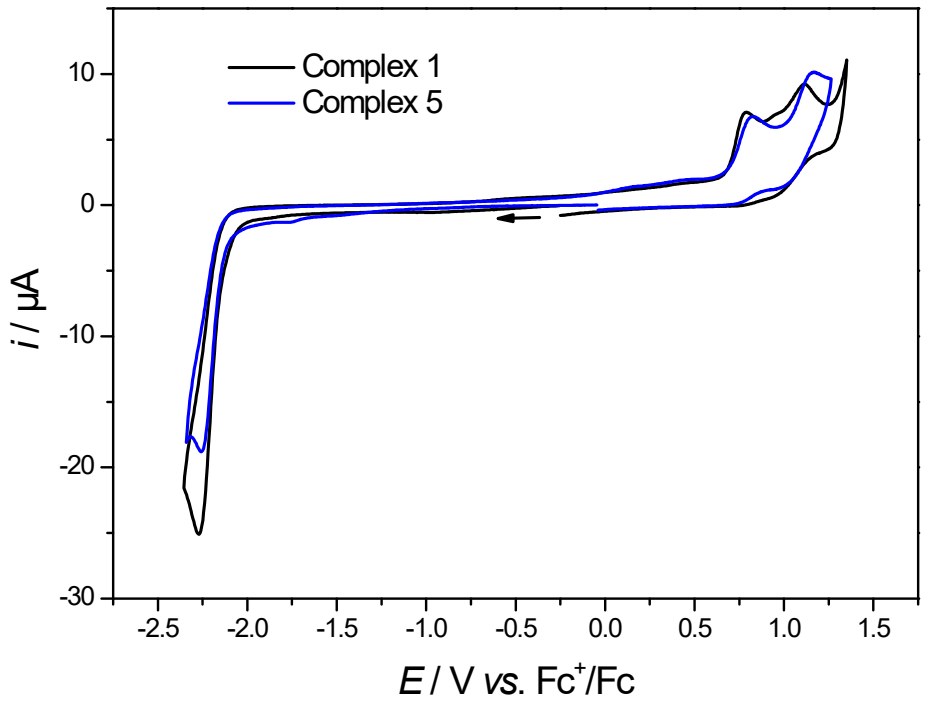


Fig. S66. Cyclic voltammograms of complexes **1** (black) and **5** (blue) at a Pt working electrode in CH_2Cl_2/NBu_4PF_6 0.1 M (*E* / V *vs.* Fc^+/Fc, v = 0.1 V s^{-1}, C = 0.5 mM). The arrow indicates the scanning direction from the initial potential.

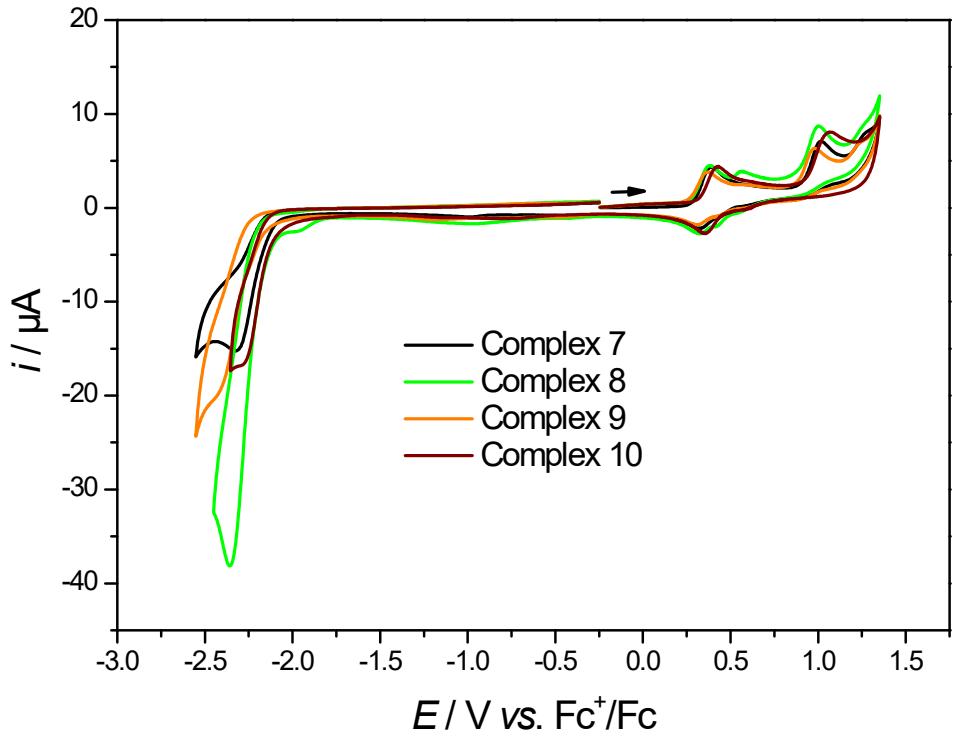


Fig. S67. Cyclic voltammograms of complexes **7** (black), **8** (green), **9** (orange) and **10** (brown) at a Pt working electrode in CH_2Cl_2/NBu_4PF_6 0.1 M (*E* / V *vs.* Fc^+/Fc, *v* = 0.1 V s^{-1}, *C* = 0.5 mM). The arrow indicates the scanning direction from the initial potential.

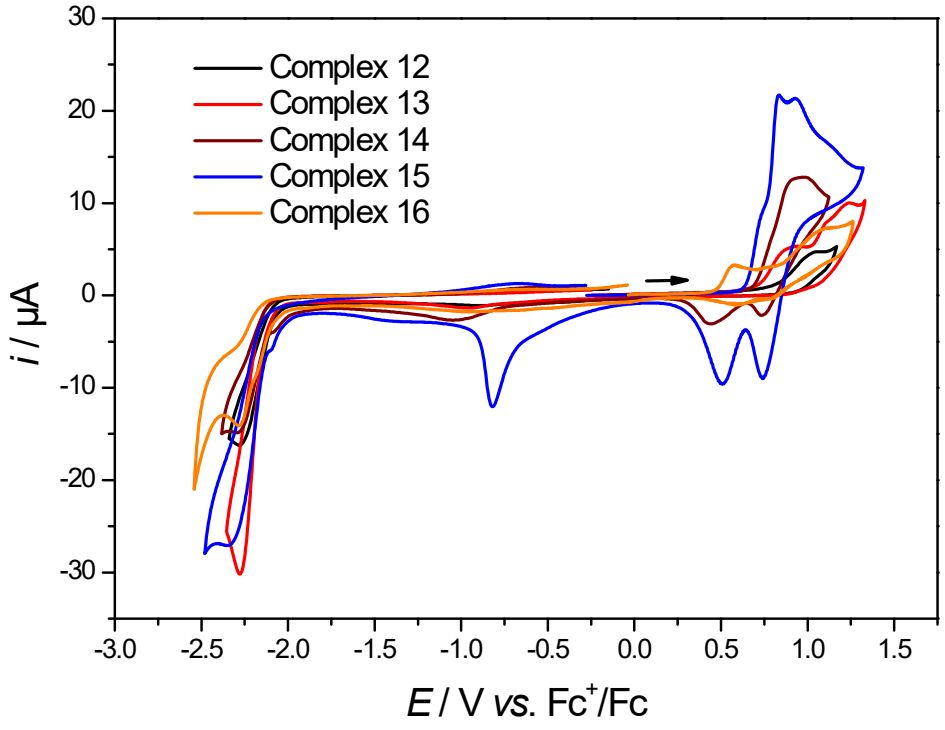


Fig. S68. Cyclic voltammograms of complexes **12** (black), **13** (red), **14** (brown), **15** (blue) and **16** (orange) at a Pt working electrode in CH_2Cl_2/NBu_4PF_6 0.1 M (E / V *vs.* Fc^+/Fc, v = 0.1 V s^{-1}, C = 0.5 mM). The arrow indicates the scanning direction from the initial potential.

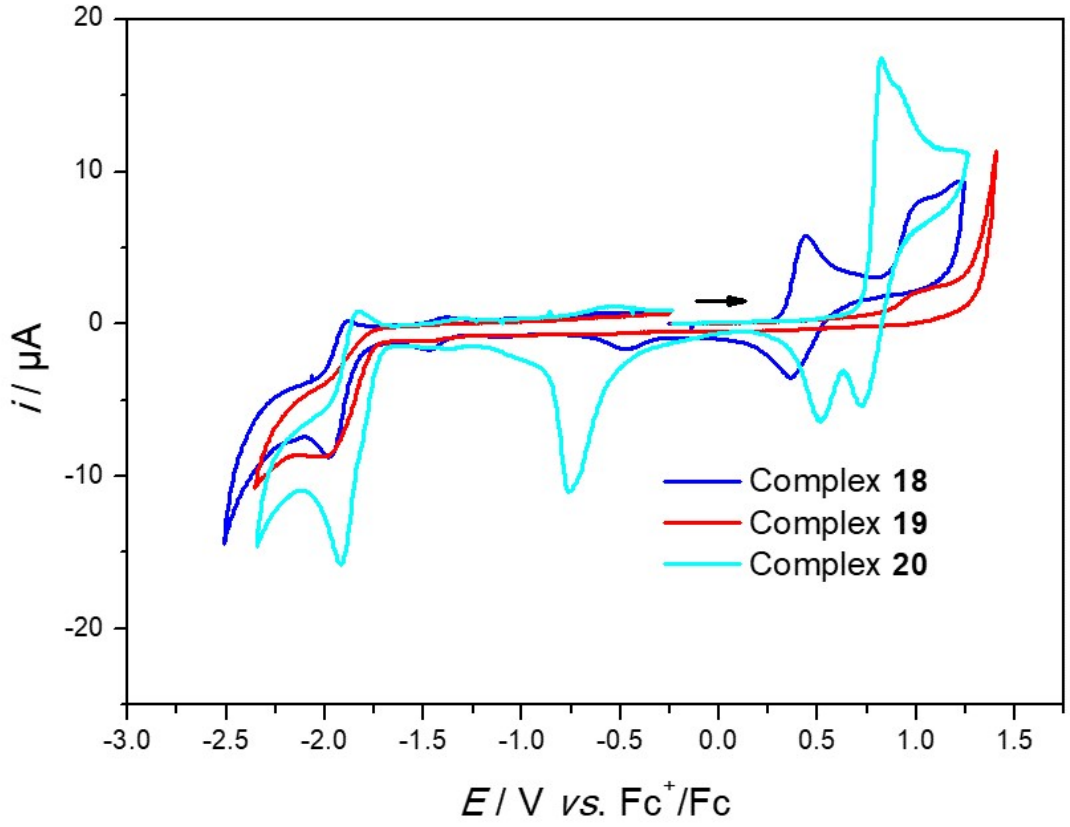


Fig. S69. Cyclic voltammograms of complexes **18** (blue), **19** (red) and **20** (cyan) at a Pt working electrode in CH_2Cl_2/NBu_4PF_6 0.1 M (*E* / V *vs.* Fc^+/Fc, v = 0.1 V s^{-1}, C = 0.5 mM). The arrow indicates the scanning direction from the initial potential.

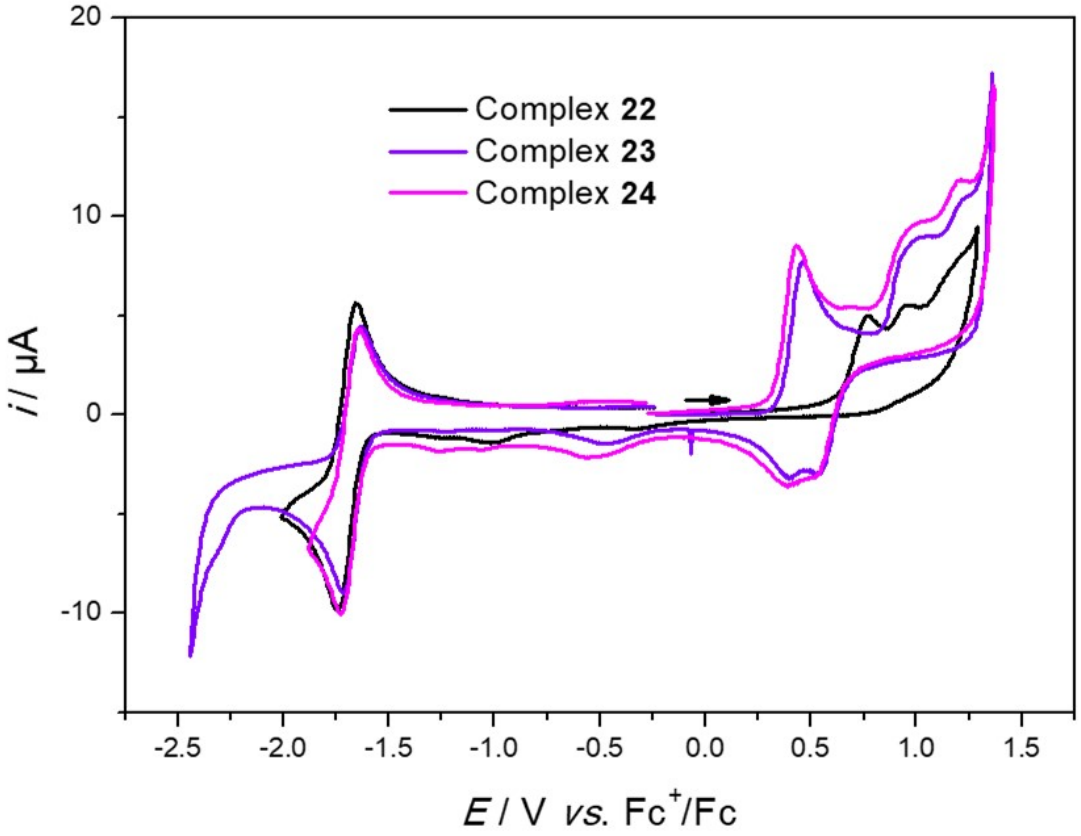


Fig. S70. Cyclic voltammograms of complexes **22** (black), **23** (blue) and **24** (pink) at a Pt working electrode in CH_2Cl_2/NBu_4PF_6 0.1 M (E / V *vs.* Fc^+/Fc, v = 0.1 V s^{-1}, C = 0.5 mM). The arrow indicates the scanning direction from the initial potential.

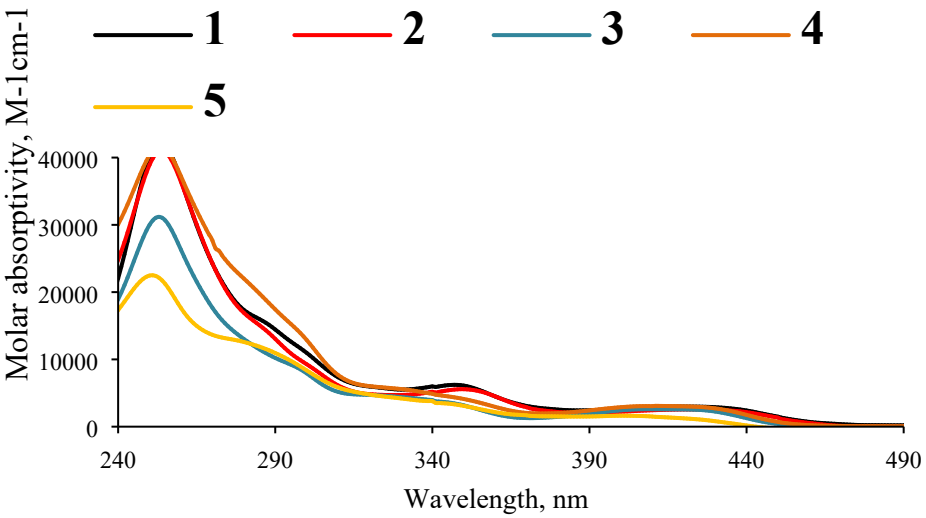


Fig. S71: Absorption spectra of phenylpyrimidine complexes **1-5** in DCM solution (C ~ 10^{-5} M).

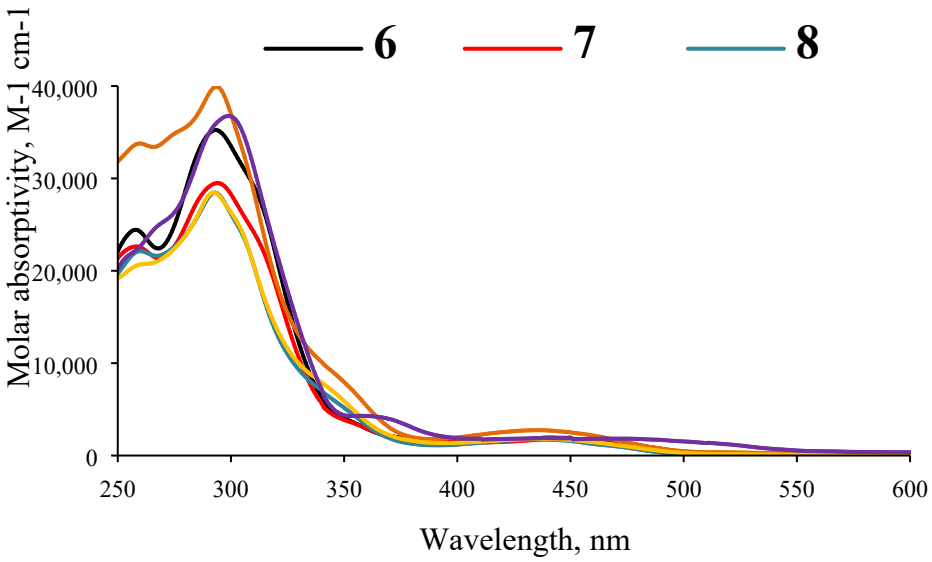


Fig. S72: Absorption spectra of phenylpyrimidine complexes **6 – 11** in DCM solution (C ~ 10^{-5} M).

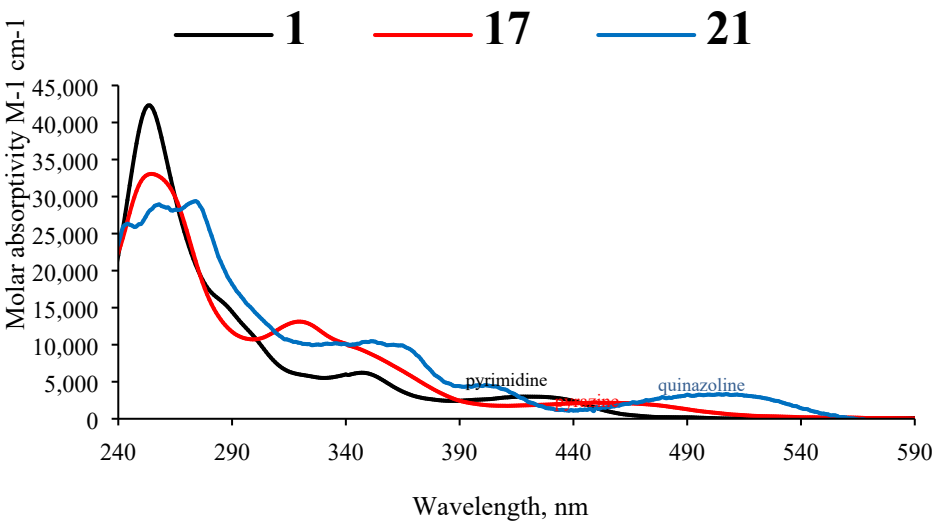


Fig. S73: Absorption spectra of methoxy complexes **1, 17** and **21** in DCM solution (C ~ 10^{-5} M).

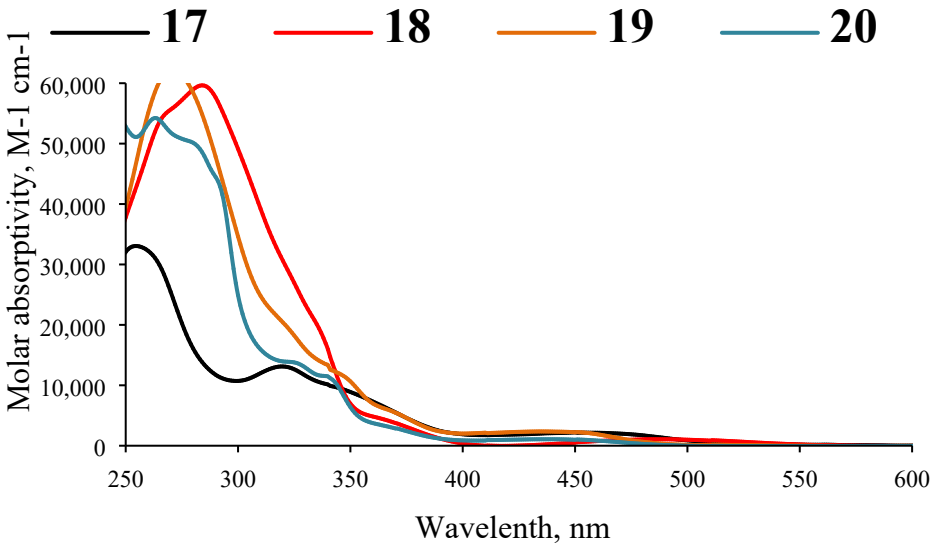


Fig. S74: Absorption spectra of phenylpyrazine complexes **17 – 20** in DCM solution (C ~ 10^{-5} M).

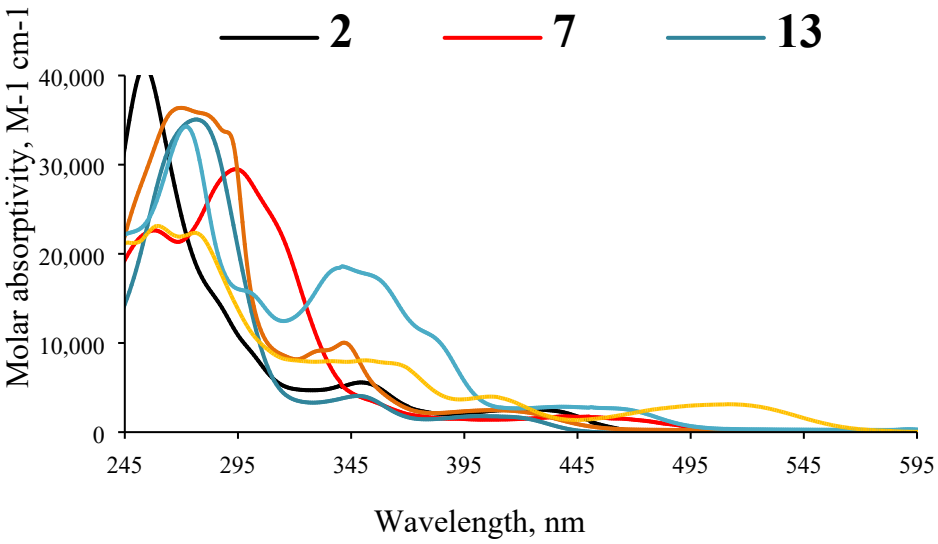


Fig. S75: Absorption spectra of phenylpyrimidine complexes **2, 7, 13, 15, 16** and **22** in DCM solution (C ~ 10^{-5} M).

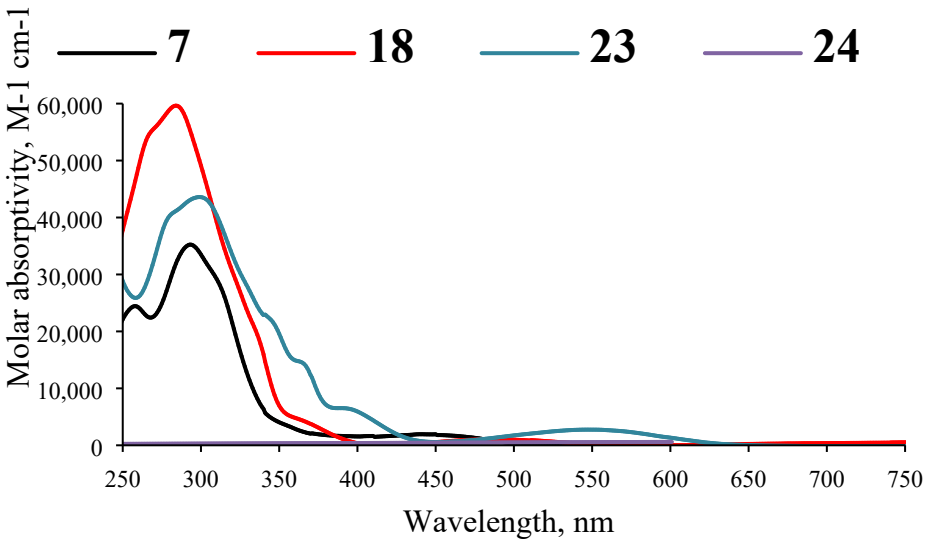


Fig. S76: Absorption spectra of diphenylamino-complexes **7, 19, 23** and **24** in DCM solution (C ~ 10^{-5} M).

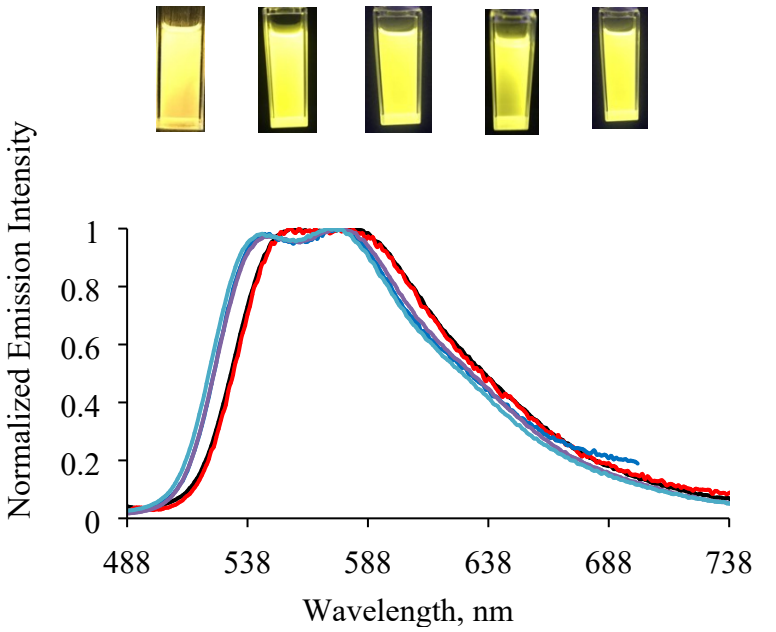


Fig. S77: Normalized Emission spectra of phenylpyrimidine complexes **1-5** in deoxygenated DCM solution (C ~ 10^{-5} M). $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band. Inset: picture of DCM solution taken under UV irradiation.

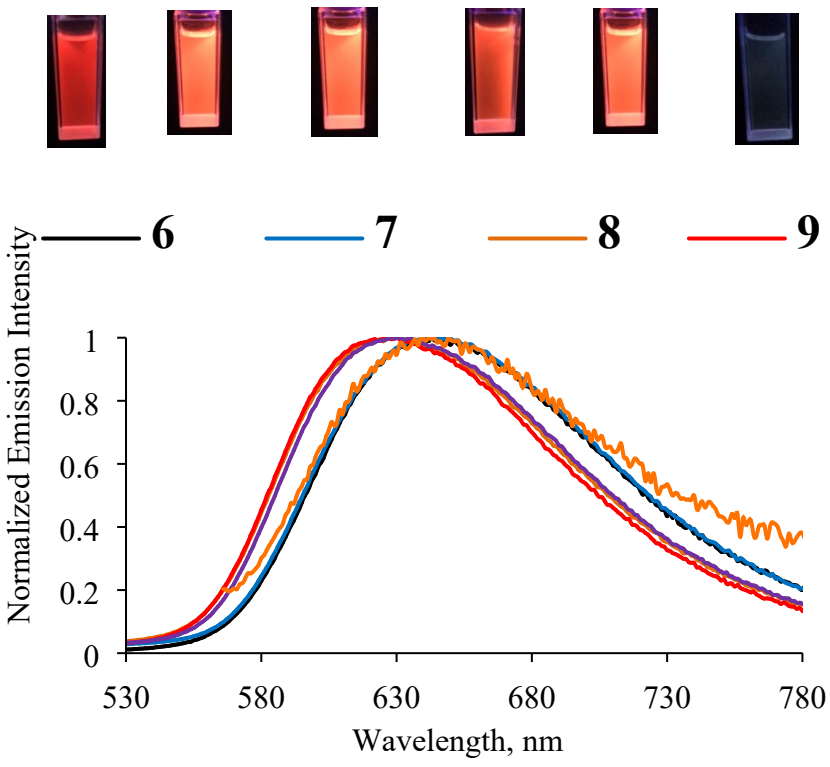


Fig. S78: Normalized Emission spectra of phenylpyrimidine complexes **6-11** in deoxygenated DCM solution (C ~ 10^{-5} M). $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band. Inset: picture of DCM solution taken under UV irradiation.

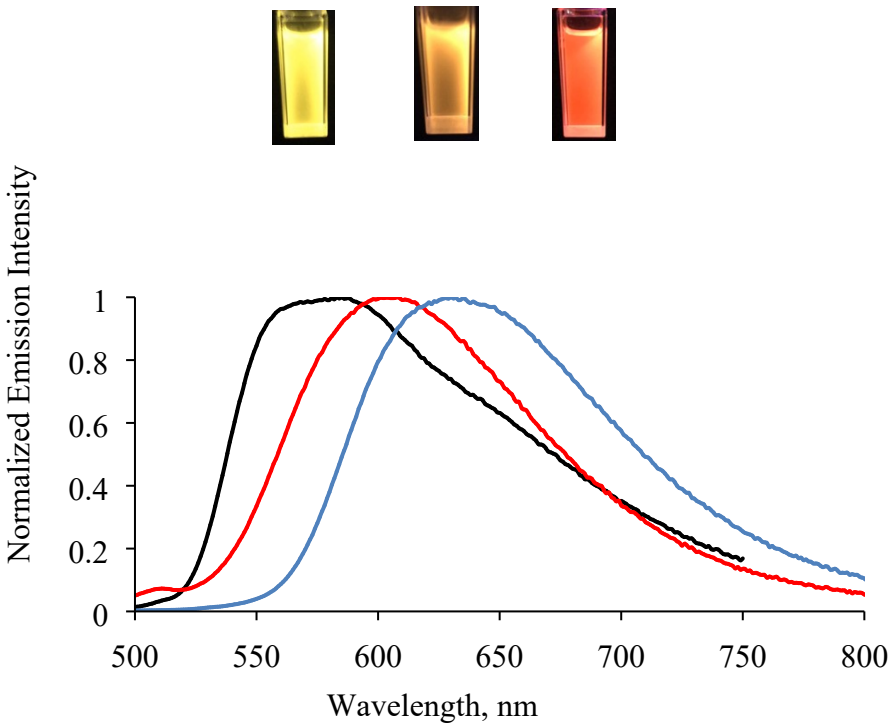


Fig. S79: Normalized Emission spectra of phenylpyrazine complexes **17, 19** and **20** in deoxygenated DCM solution (C ~ 10^{-5} M). $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band. Inset: picture of DCM solution taken under UV irradiation.

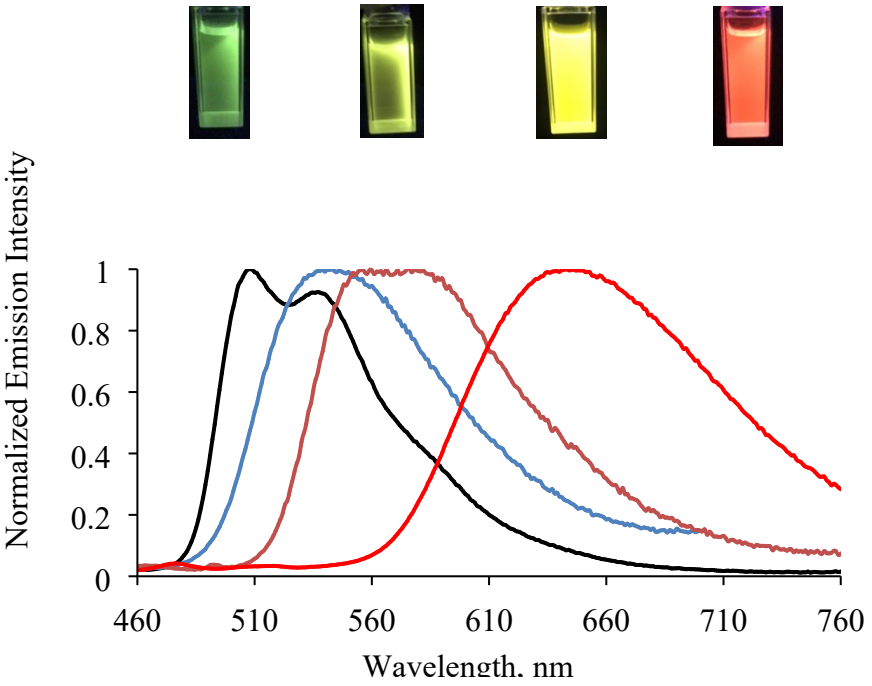


Fig. S80: Normalized Emission spectra of phenylpyrimidine complexes **2, 7, 13** and **15** in deoxygenated DCM solution (C ~ 10^{-5} M). $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band. Inset: picture of DCM solution taken under UV irradiation.

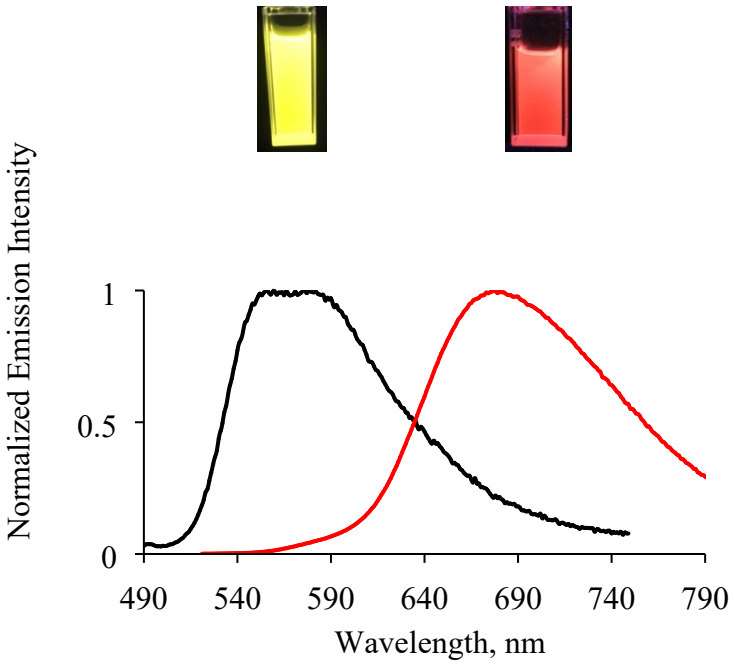


Fig. S81: Normalized Emission spectra of phenyldiazine complexes **2** and **22** in deoxygenated DCM solution (C ~ 10^{-5} M). $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band. Inset: picture of DCM solution taken under UV irradiation.

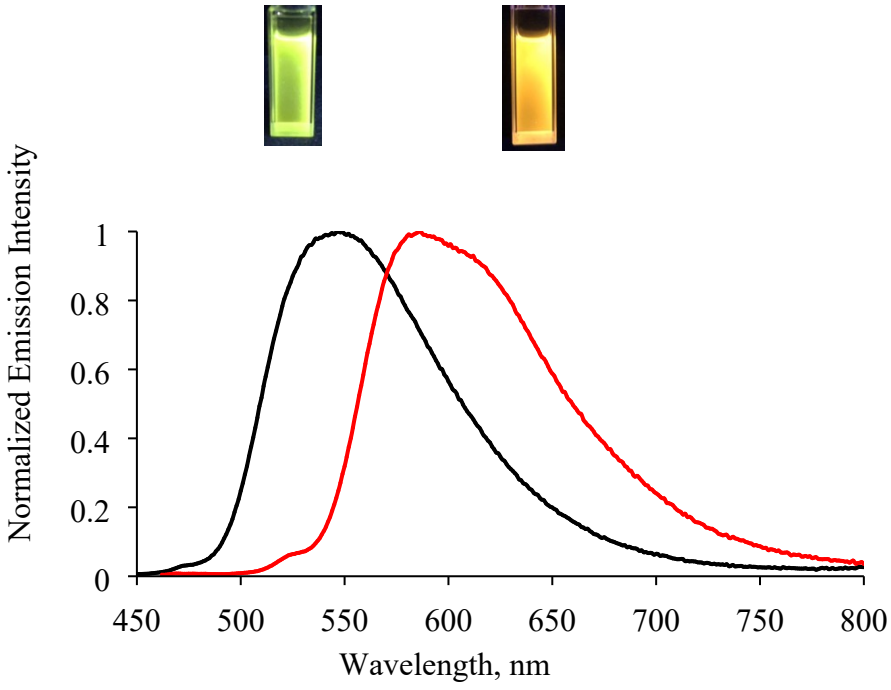


Fig. S82: Normalized Emission spectra of complexes **14** and **16** in deoxygenated DCM solution (C ~ 10^{-5} M). $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band. Inset: picture of DCM solution taken under UV irradiation.

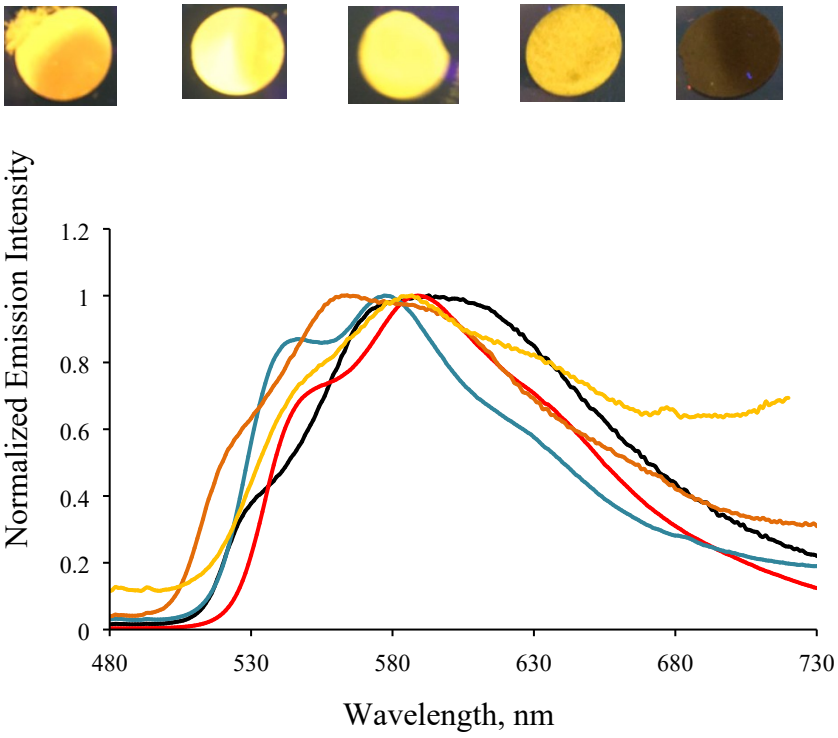


Fig. S83: Solid state emission (2 w% in KBr matrix) of complexes **1-5.** $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation.

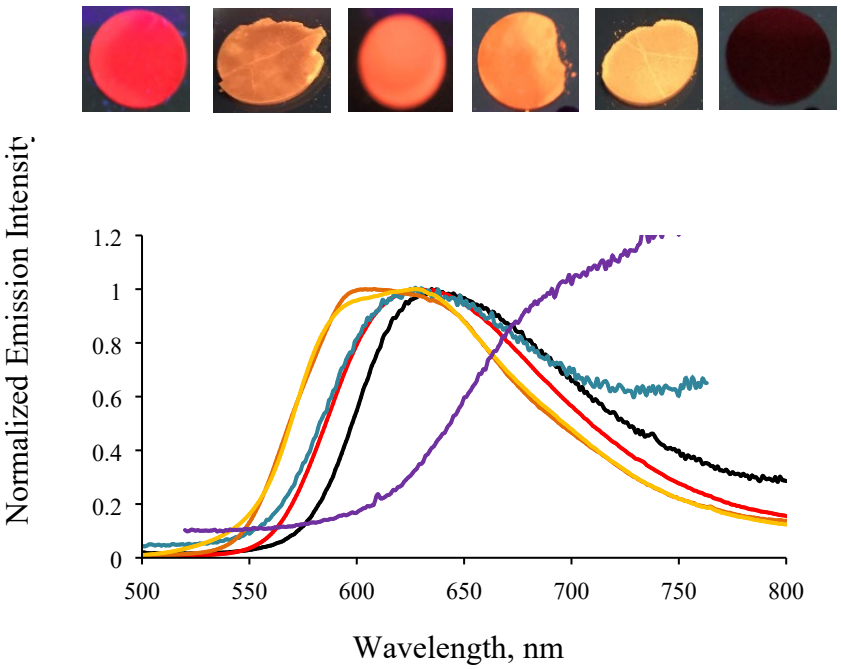


Fig. S84: Solid state emission (2 w% in KBr matrix) of complexes **6-11**. $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation

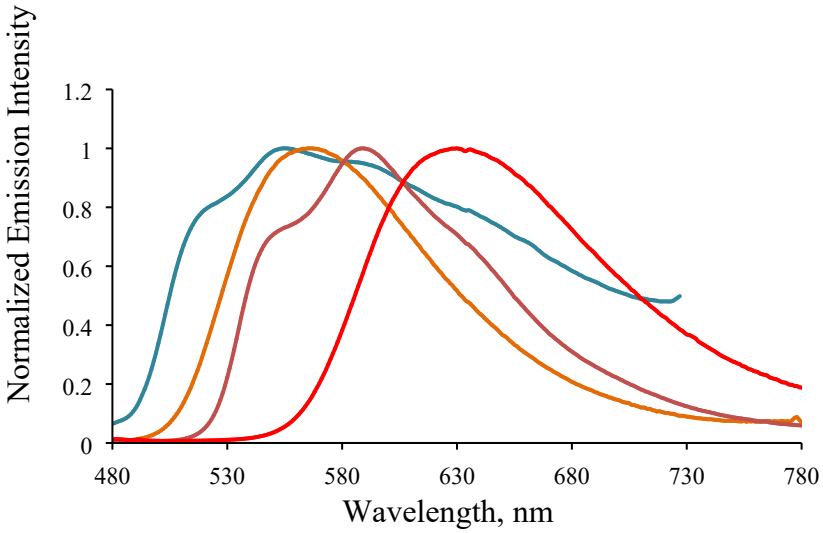


Fig. S85: Solid state emission (2 w% in KBr matrix) of complexes **2, 7, 13** and **15.** $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation.

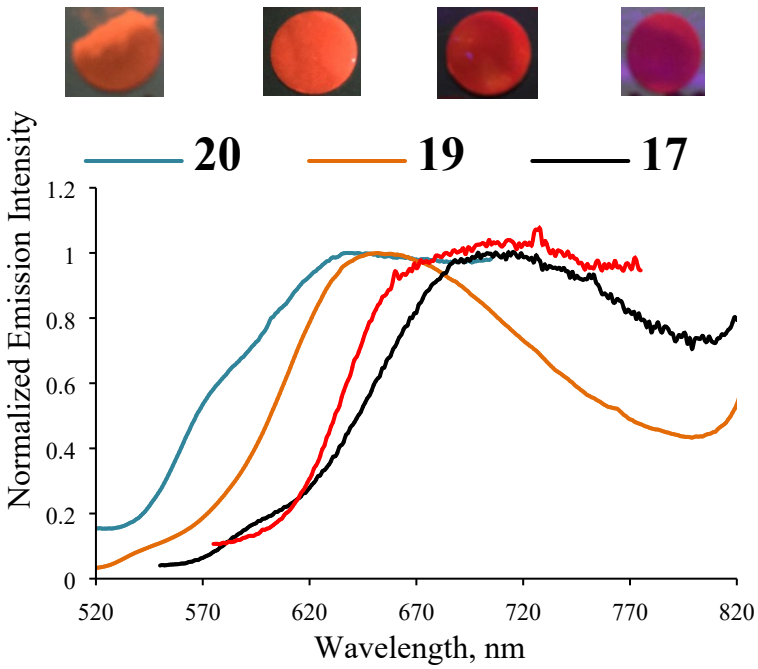
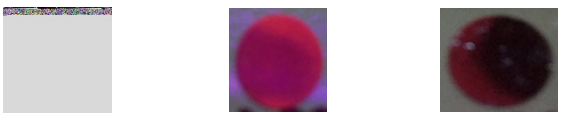


Fig. S86: Solid state emission (2 w% in KBr matrix) of complexes **17-20.** $\lambda_{exc} = \lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation.



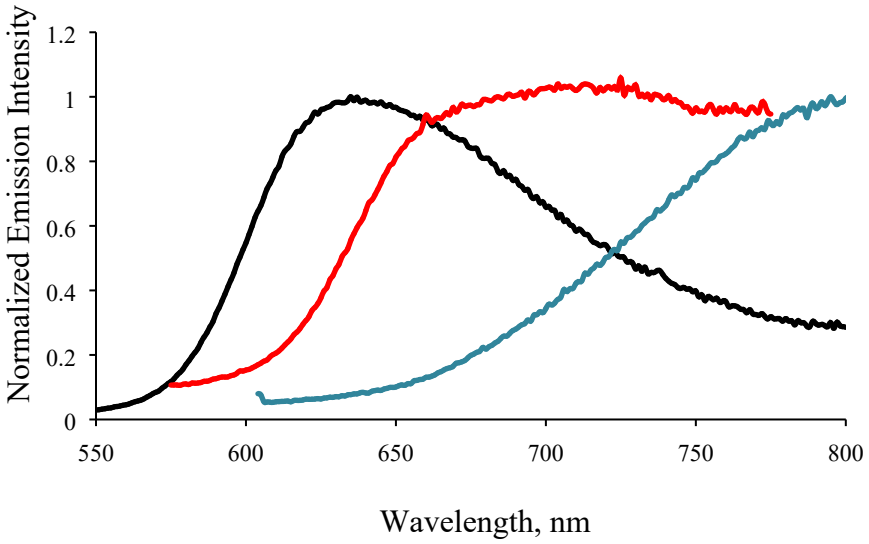


Fig. S87: Solid state emission (2 w% in KBr matrix) of complexes **6, 18** and **23**. λ_{exc} = $\lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation.

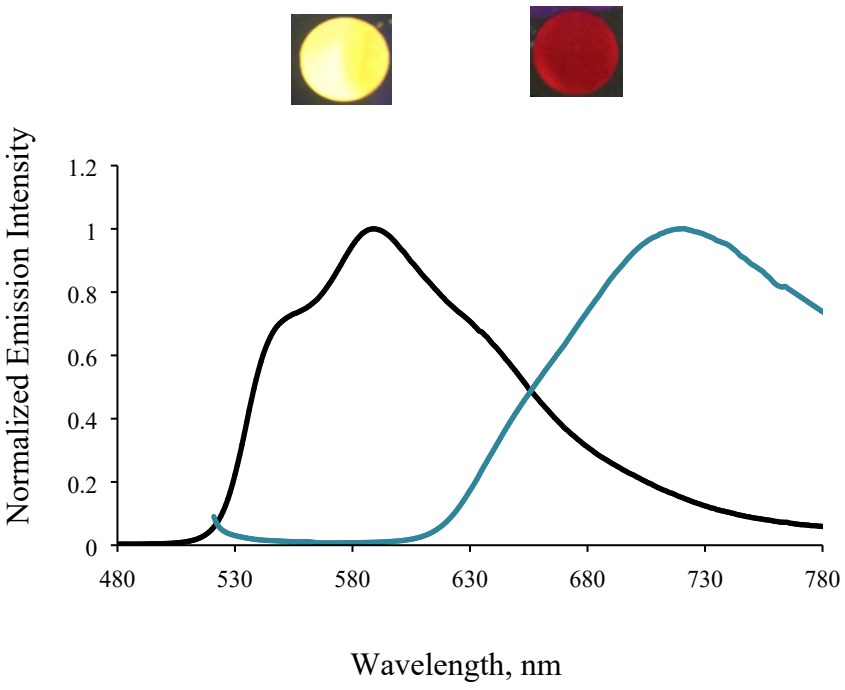
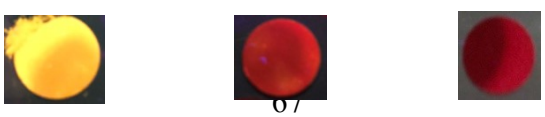


Fig. S88: Solid state emission (2 w% in KBr matrix) of complexes **2** and **23.** λ_{exc} = $\lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation.



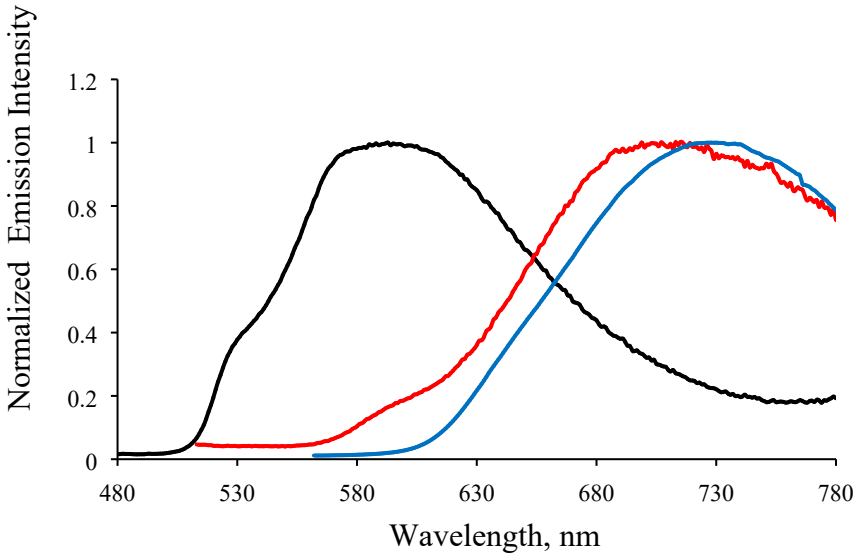


Fig. S89: Solid state emission (2 w% in KBr matrix) of complexes **1, 17** and **21.** λ_{exc} = $\lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation

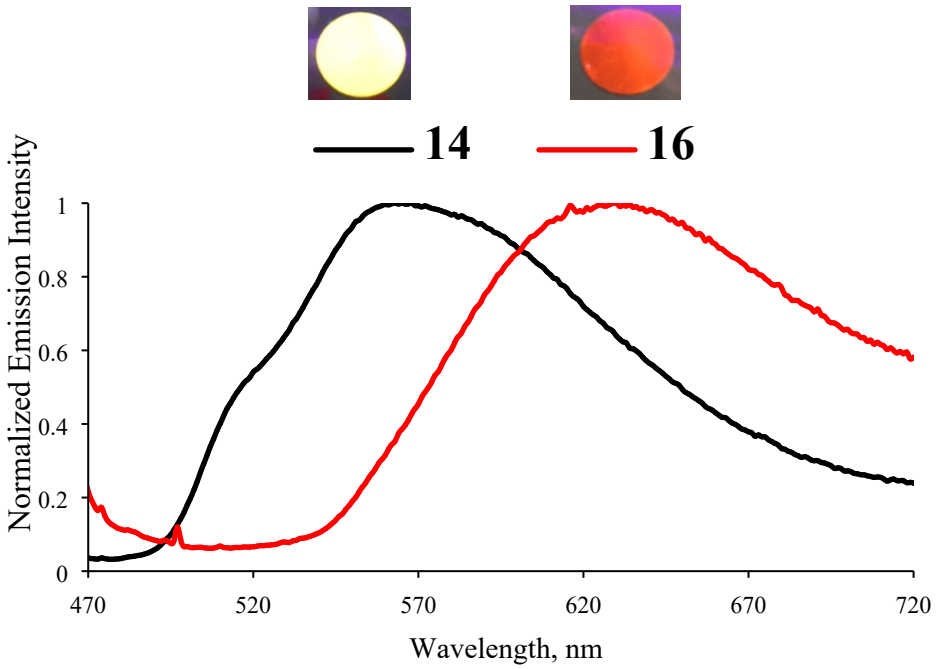


Fig. S90: Solid state emission (2 w% in KBr matrix) of complexes **14** and **16.** λ_{exc} = $\lambda^{abs}{}_{max}$ of the lowest energy band in DCM solution Inset: picture of KBr pellets taken under UV irradiation.

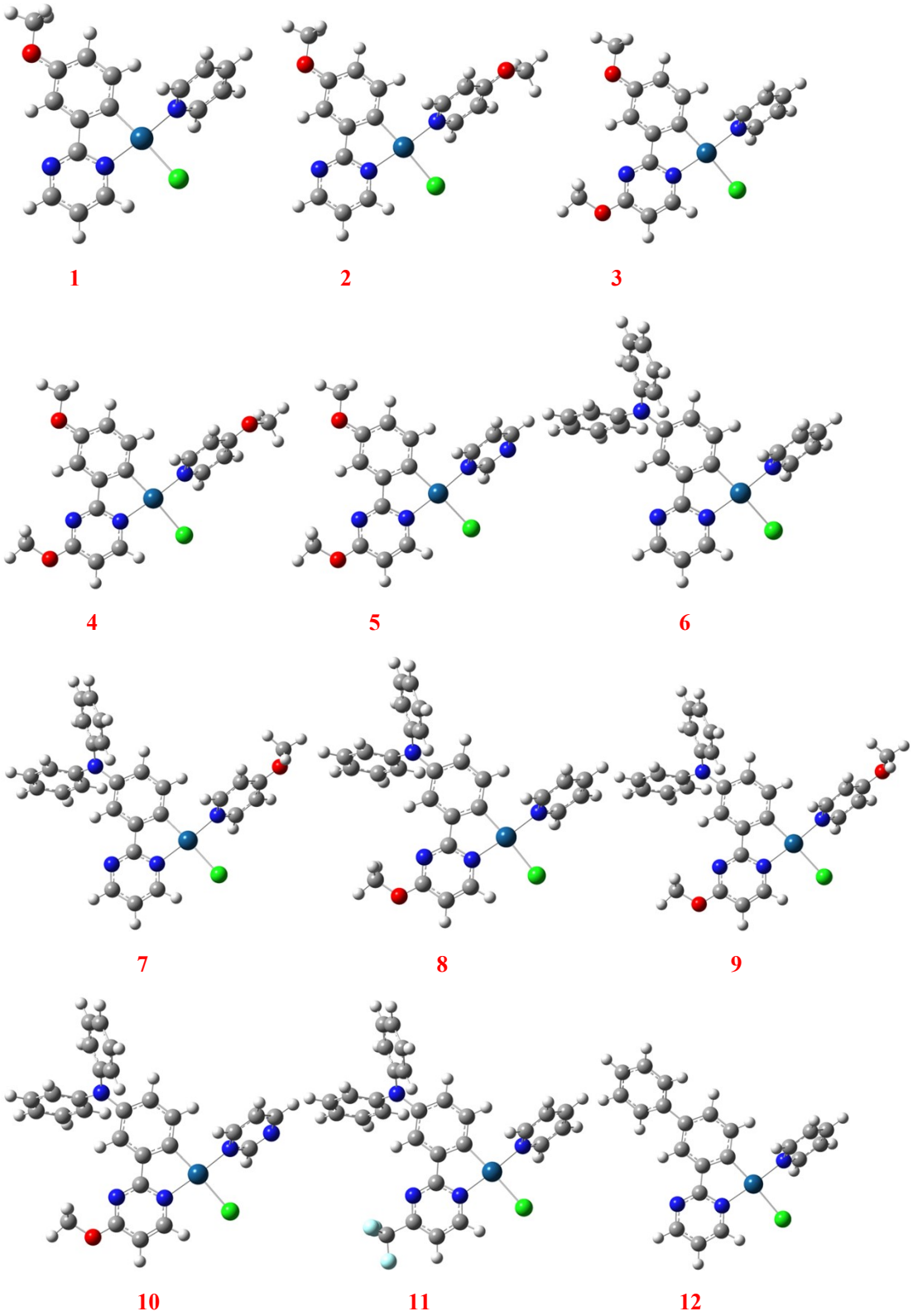


Fig. S91. DFT-optimized structures of complexes **1-12**.

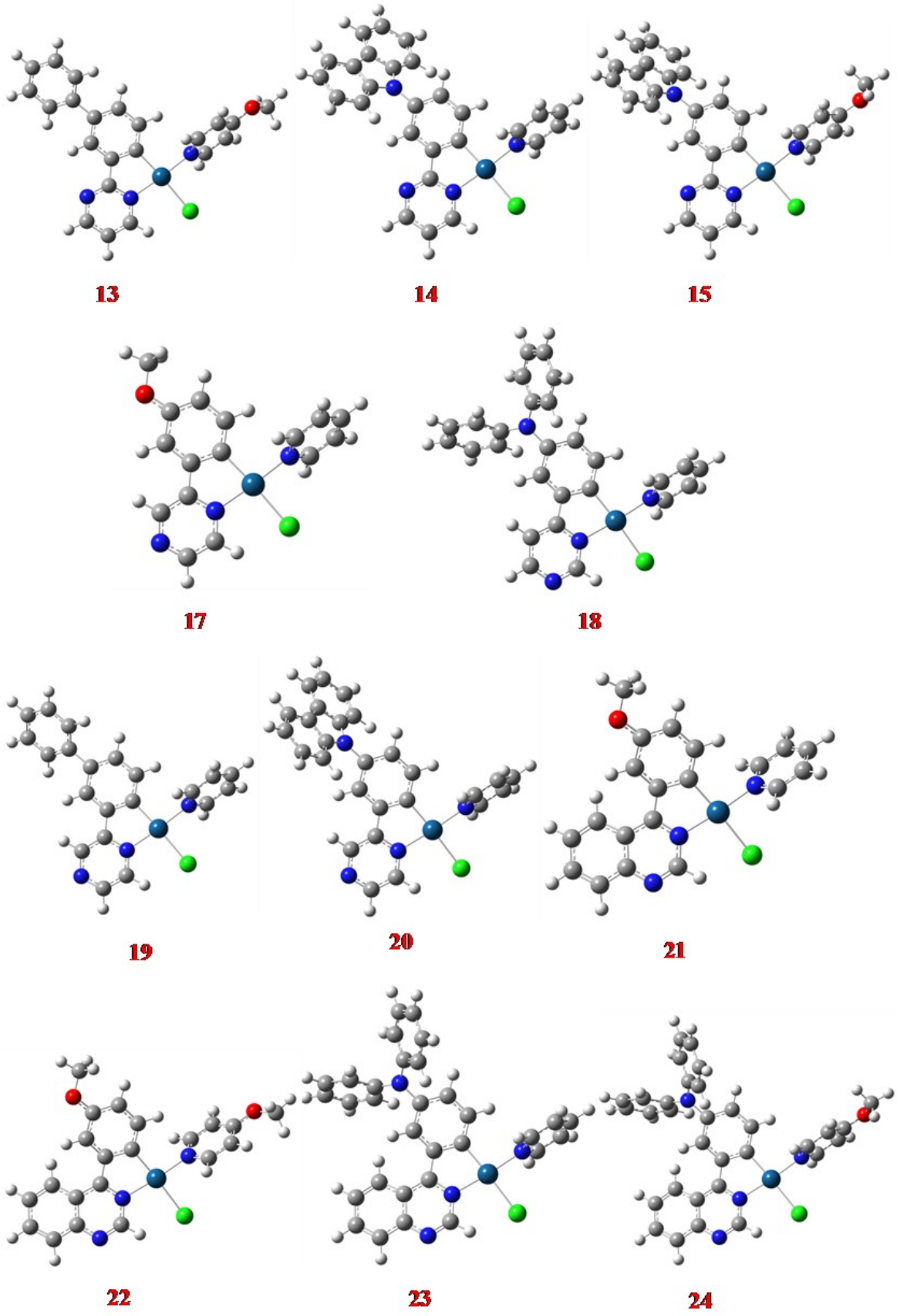


Fig. S92. DFT-optimized structures of complexes **13**-**15** and **17**-**24**.

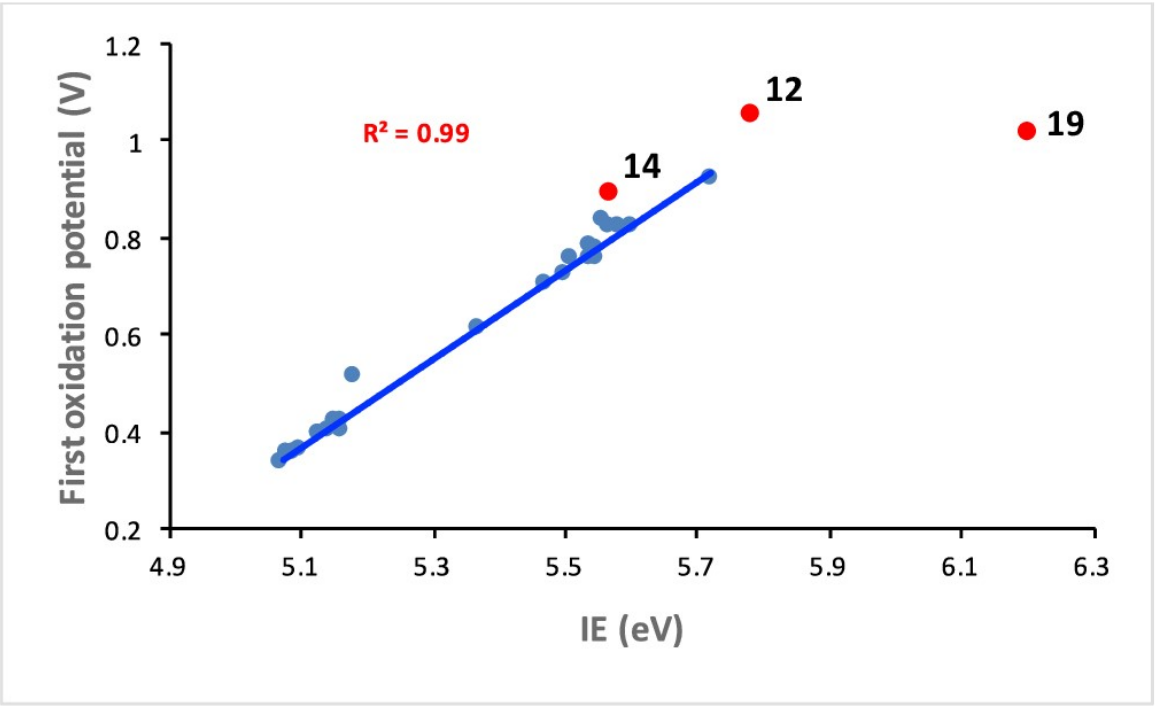


Fig. S93. The linear correlation between the first recorded oxidation peak and the computed ionization energies for a series of 23 complexes (see text). Complexes **12**, **14** and **19** (not included in the fit) are added for comparison.

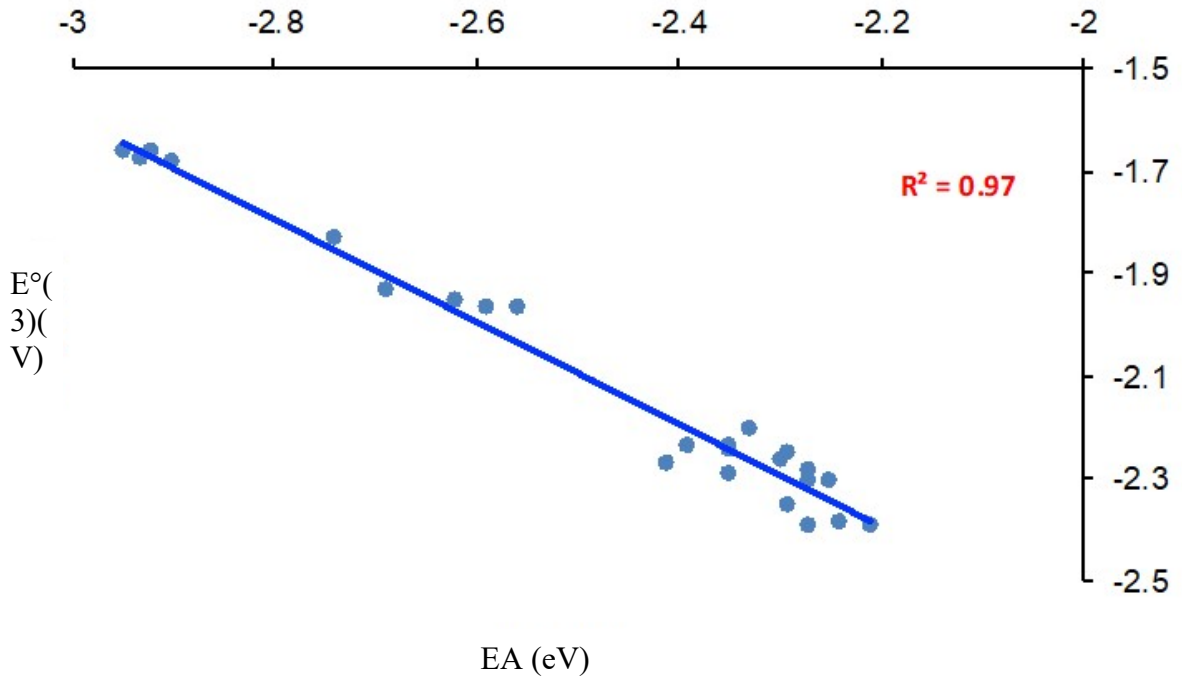


Fig. S94. The linear correlation between the recorded $E^0(3)$ reduction potentials and the computed electron affinities for a series of 24 complexes.

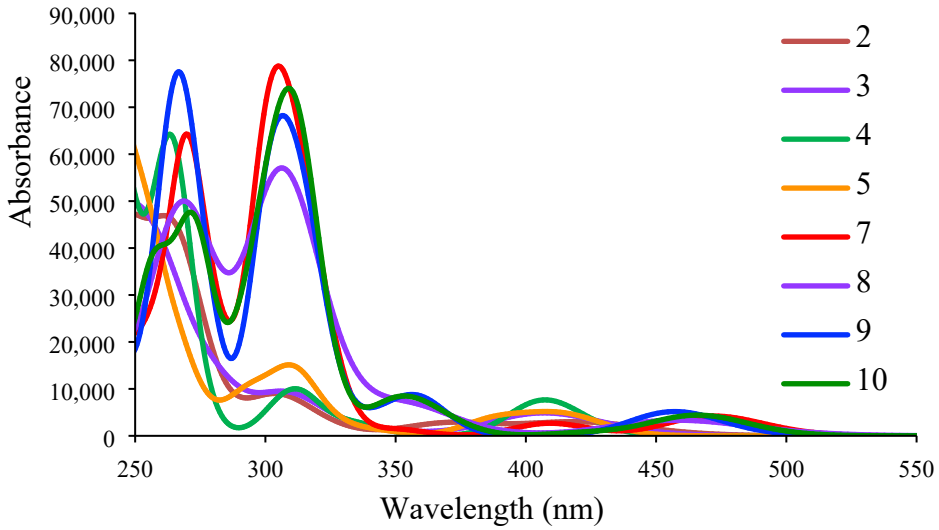


Fig. S95. TD-DFT-simulated UV-vis spectra of complexes **2-5**, **7-10**.

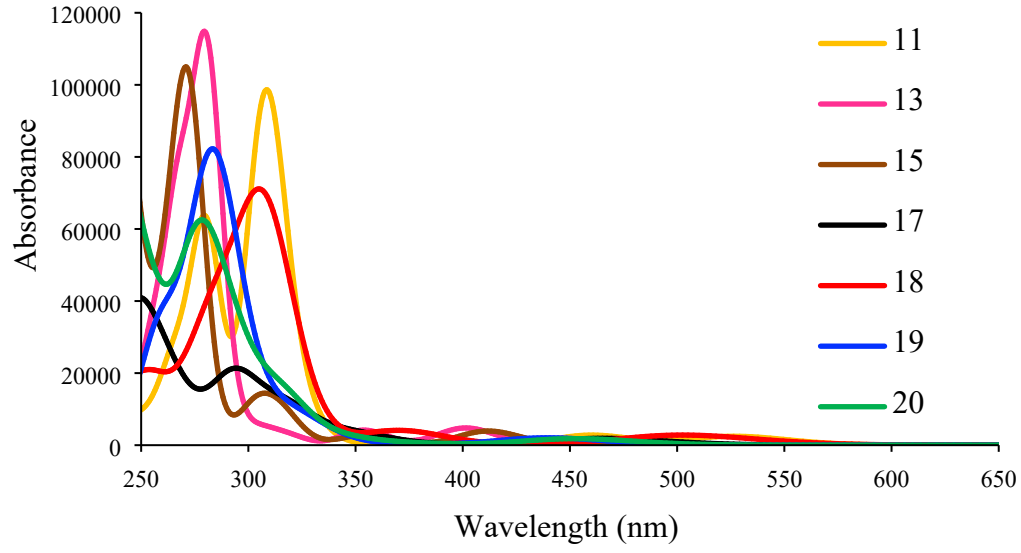


Fig. S96. TD-DFT-simulated UV-vis spectra of complexes **11**, **13**, **15**, **17-20**.

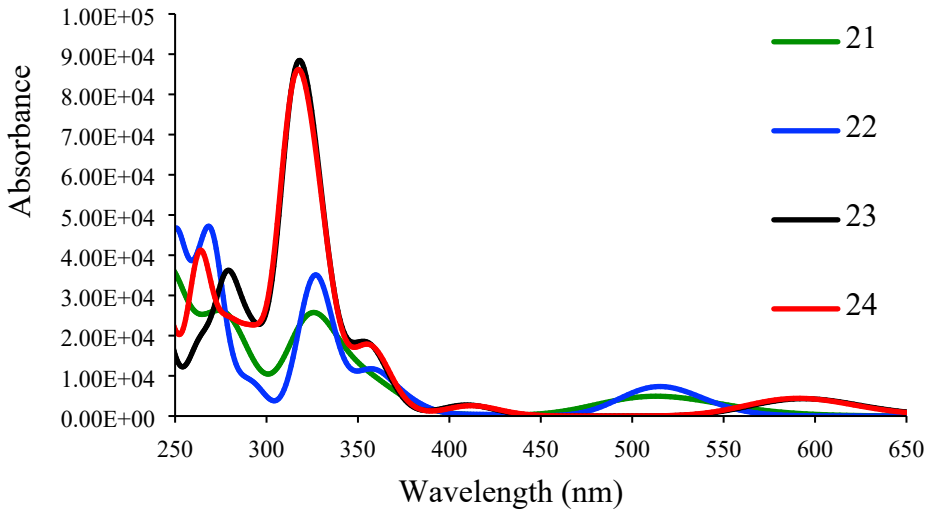


Fig. S97. TD-DFT-simulated UV-vis spectra of complexes **21**-**24.**

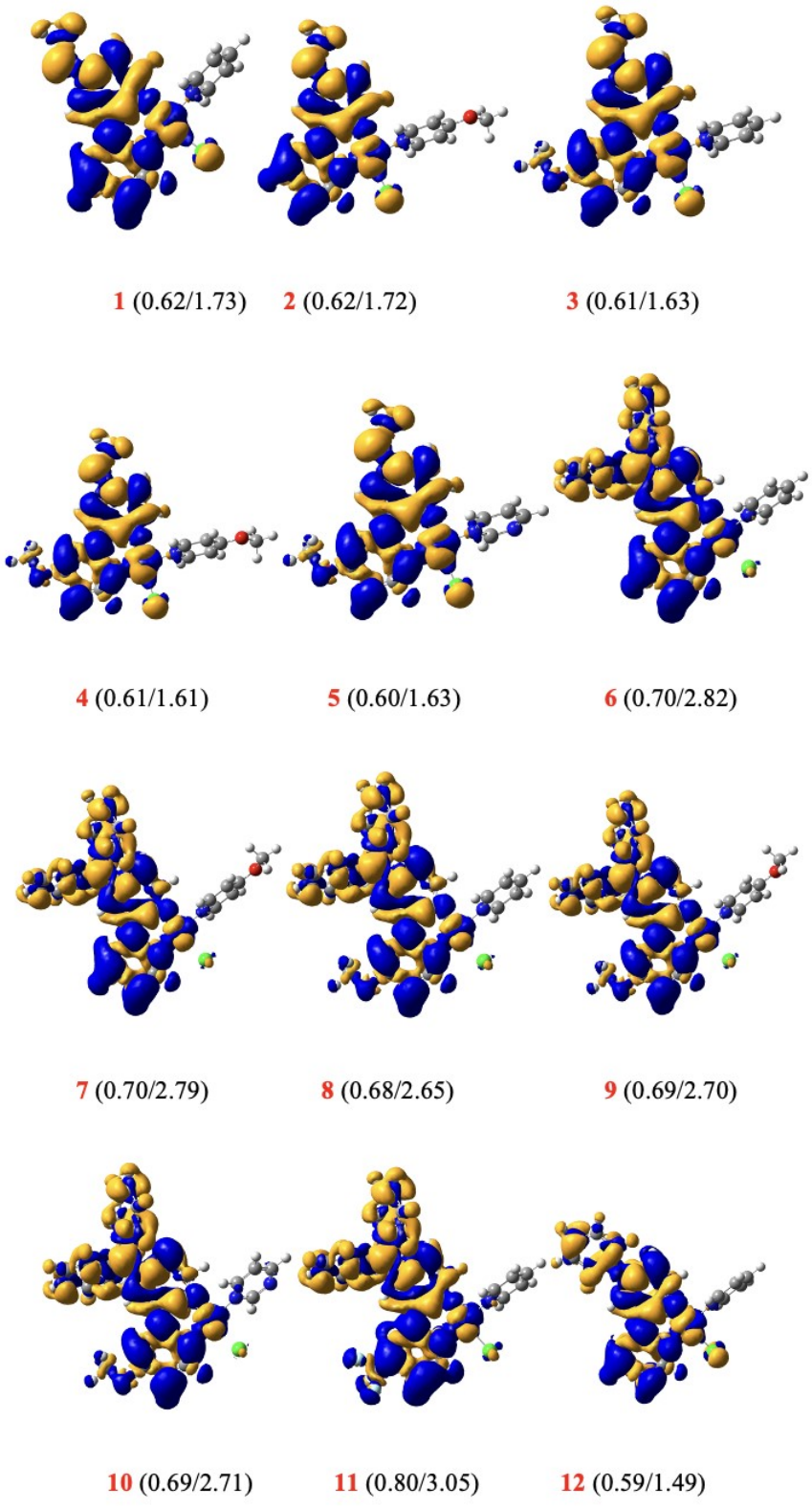


Fig. S98. Density difference plots associated with the triplet→singlet emissive transitions for complexes **1**-**12**. The blue and yellow colors indicate an increase and decrease of density upon de-excitation, respectively. The numerical values are the computed charge transfers (q^{CT}) and corresponding distance transfer (d^{CT}, in Å), respectively (see Computational details)

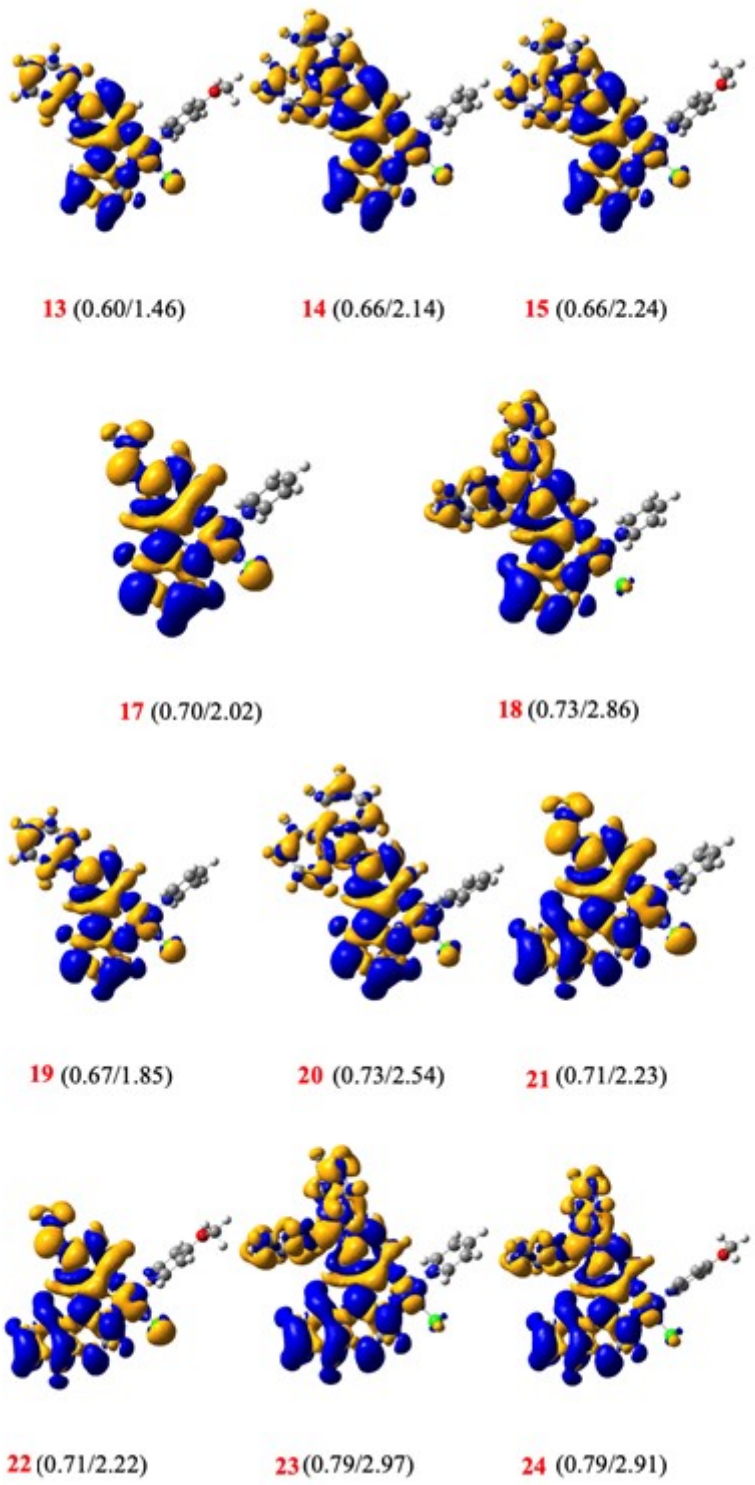


Fig. S99. Density difference plots associated with the triplet→singlet emissive transitions for complexes **13**-**15**, **17**-**24**. The blue and yellow colors indicate an increase and decrease of density upon de-excitation, respectively. The numerical values are the computed charge transfers (q^{CT}) and corresponding distance transfer (d^{CT}, in Å), respectively (see Computational details).

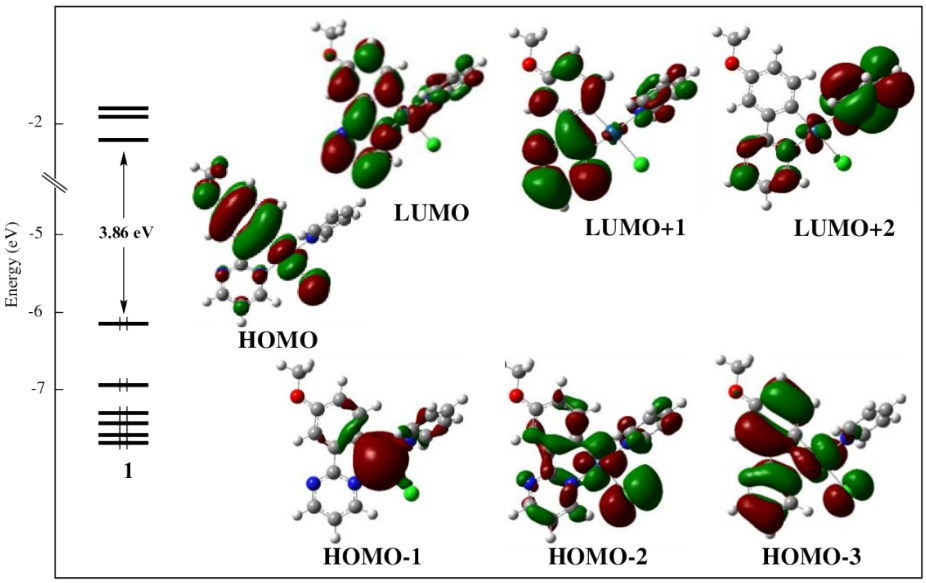


Fig. S100. Kohn-Sham MO diagrams of complex **1**.

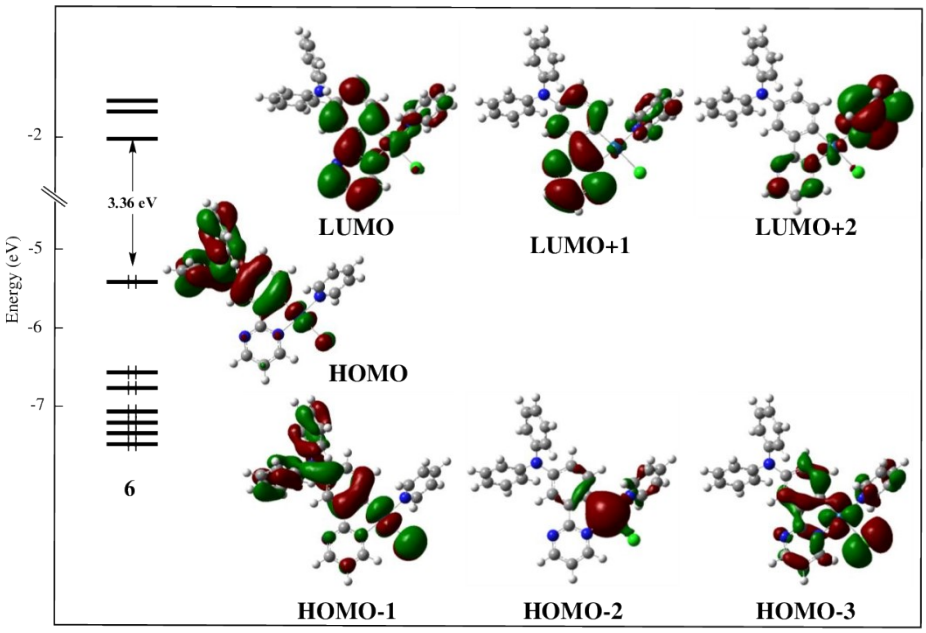


Fig. S101. Kohn-Sham MO diagrams of complex **6**.

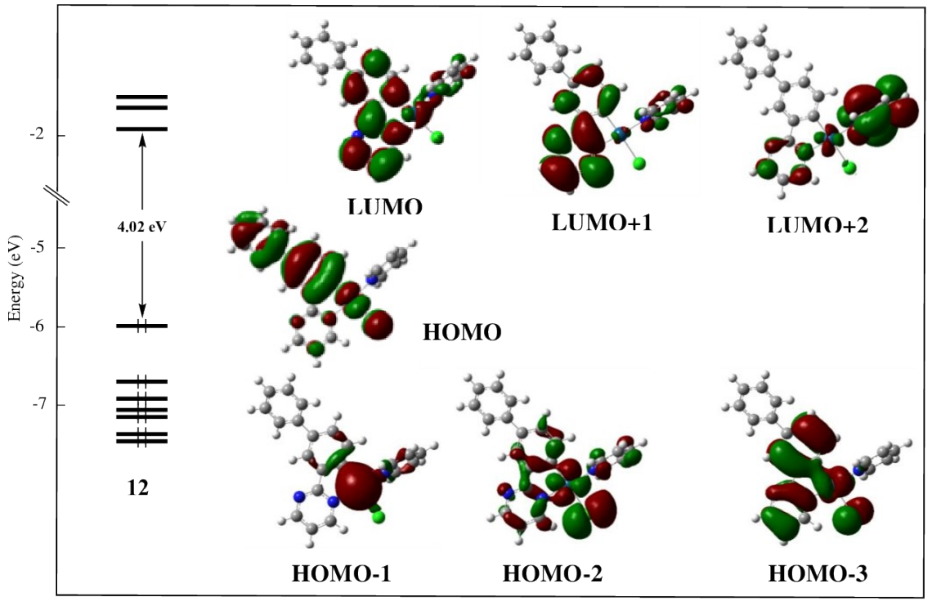


Fig. S102. Kohn-Sham MO diagrams of complex **12**.

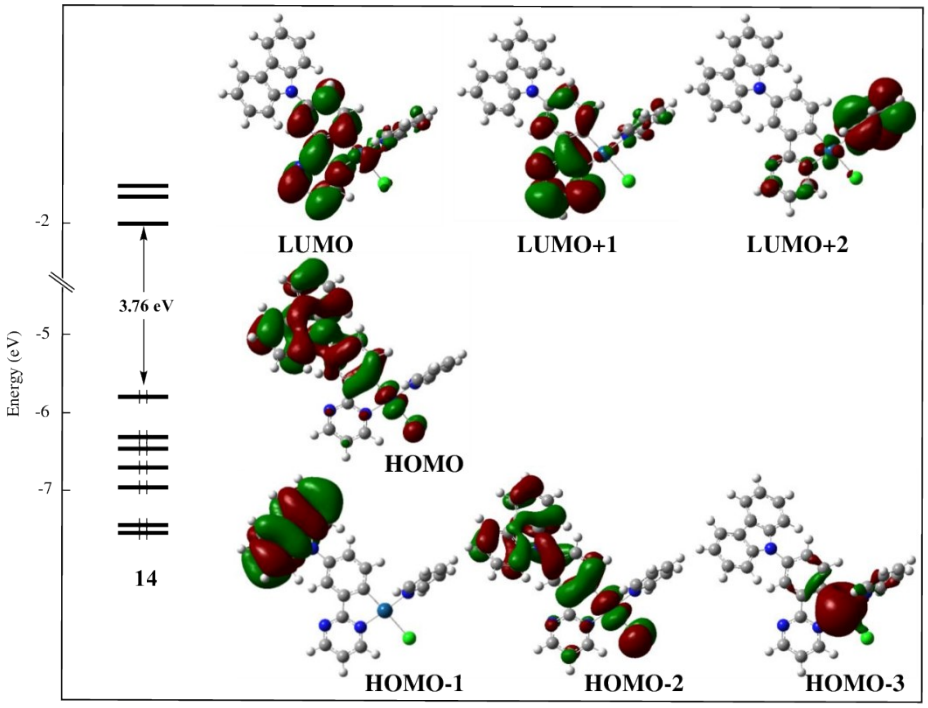


Fig. S103. Kohn-Sham MO diagrams of complex **14**.

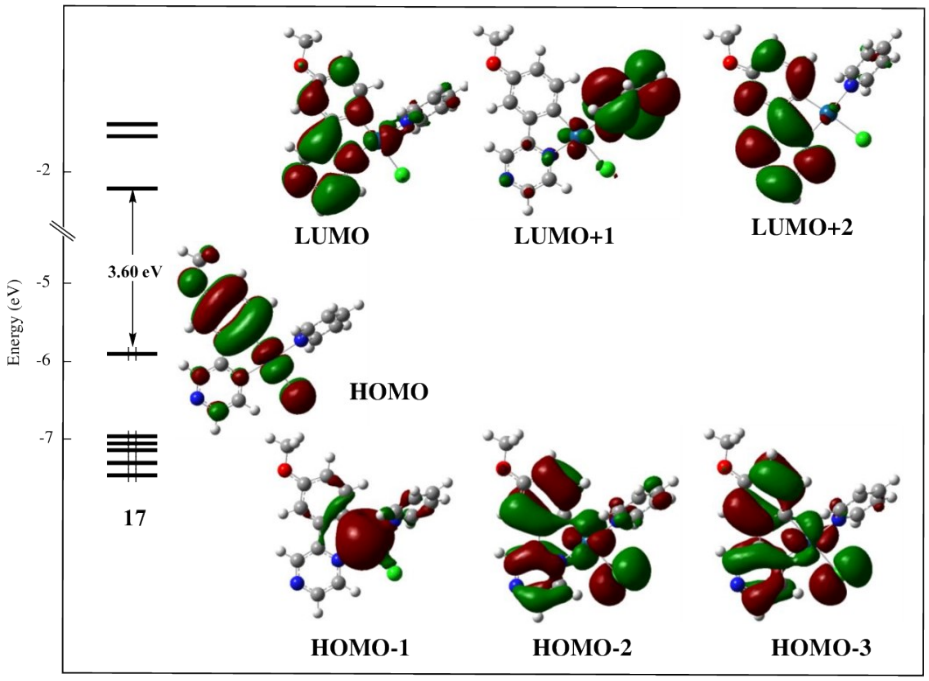


Fig. S104. Kohn-Sham MO diagrams of complex **17**.

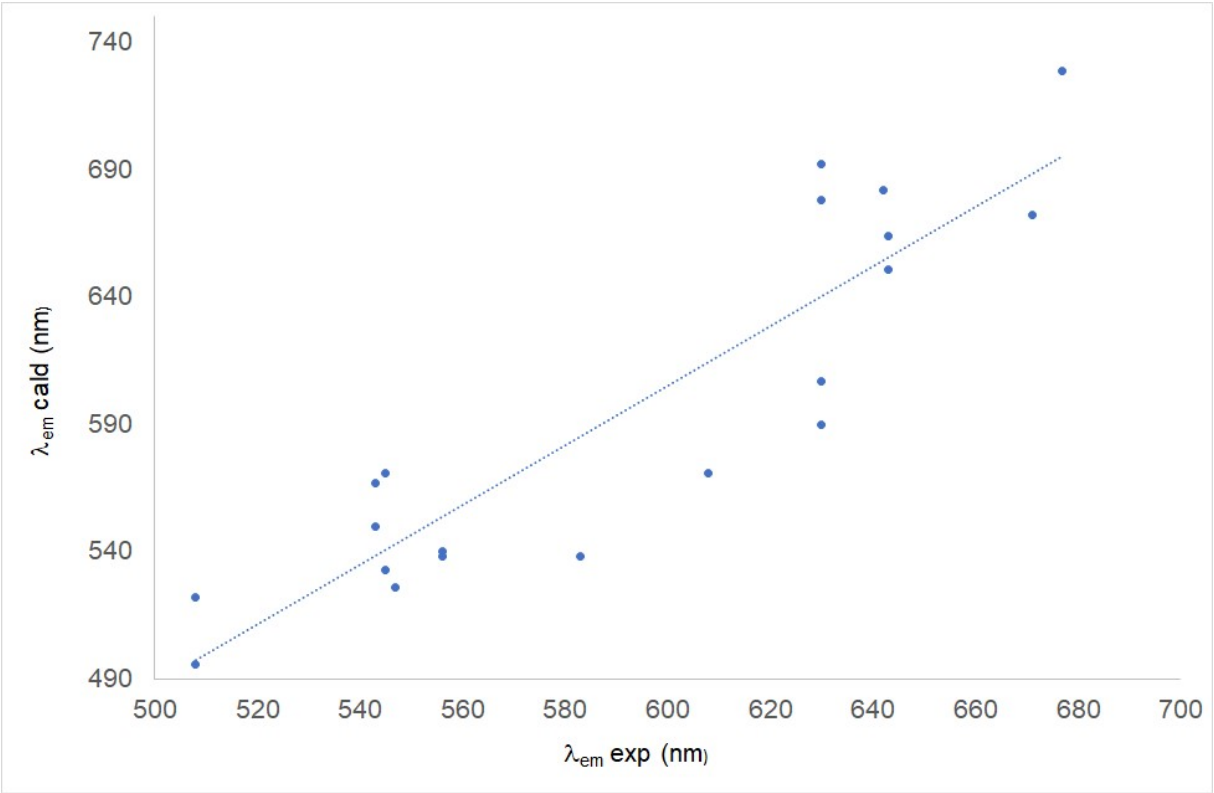


Fig. S105. Correlation between calculated and experimental phosphorescence maxima

Cartesian coordinates (Å)

Comp 1

Pt	2.627012	2.708132	8.889426
Cl	3.090737	3.623759	6.696124
N	3.206907	4.353088	9.906602
N	3.408012	5.275707	12.072158
N	1.987734	1.020545	7.971415
C	3.667141	5.482465	9.368746
H	3.742013	5.494204	8.288034
C	4.016356	6.554775	10.163612
H	4.389732	7.471167	9.728724
C	3.863302	6.397931	11.530412
H	4.114999	7.200792	12.216798
C	3.091992	4.280967	11.257775
C	2.597701	3.004373	11.742933
C	2.441733	2.740253	13.096363
H	2.673262	3.498813	13.834869
C	1.991142	1.490938	13.501453
C	1.711913	0.525079	12.536159
H	1.368975	-0.459982	12.826556
C	1.873233	0.811330	11.182422
H	1.649243	0.022313	10.473305
C	2.311459	2.055555	10.740508
C	0.697020	0.665010	8.014928
H	0.046207	1.302229	8.597853
C	0.219373	-0.450711	7.356401
H	-0.833492	-0.692407	7.418720
C	1.102035	-1.235297	6.632363
H	0.755908	-2.118719	6.109631
C	2.435970	-0.865078	6.589091
H	3.165793	-1.441621	6.036102
C	2.841273	0.270216	7.262766
H	3.868380	0.606658	7.244186
O	1.860159	1.301007	14.837514
C	1.413464	0.039182	15.283395
H	1.378258	0.095804	16.369764
H	0.412929	-0.189766	14.902476
H	2.102765	-0.757998	14.986864

Comp 2

Pt	2.527762	2.879886	8.865886
Cl	2.950319	3.911367	6.715035
N	3.223768	4.431246	9.952526
N	3.558805	5.206725	12.159357
N	1.772585	1.279496	7.876848
C	3.710694	5.572153	9.464872
H	3.739693	5.648768	8.384625
C	4.141396	6.576736	10.306966
H	4.536256	7.502242	9.912131
C	4.040348	6.340747	11.667144
H	4.357106	7.087405	12.389123
C	3.163745	4.279489	11.300880
C	2.634254	2.996785	11.729441
C	2.524951	2.654947	13.070128
H	2.820717	3.355814	13.842015
C	2.037591	1.402447	13.418488
C	1.676175	0.510987	12.409787
H	1.303344	-0.475473	12.655114
C	1.791966	0.874583	11.070084

H	1.504474	0.141544	10.324758
C	2.263777	2.125549	10.684743
C	0.473004	0.951723	7.972756
H	-0.124797	1.559929	8.637773
C	-0.083192	-0.090798	7.276446
H	-1.135842	-0.318868	7.378577
C	0.724192	-0.856999	6.432939
C	2.072206	-0.518226	6.332427
H	2.758928	-1.060548	5.698867
C	2.543584	0.553135	7.061529
H	3.580161	0.852938	6.992820
O	1.954363	1.134744	14.745320
C	1.468098	-0.131584	15.132926
H	1.479255	-0.141250	16.221263
H	0.443513	-0.292312	14.782210
H	2.107139	-0.938310	14.759522
O	0.139047	-1.859935	5.783238
C	0.932044	-2.656077	4.913692
H	1.732577	-3.156222	5.464065
H	0.258627	-3.399619	4.495005
H	1.355431	-2.051063	4.108427

Comp 3

Pt	2.629485	2.689498	8.894367
Cl	3.104048	3.624676	6.713196
N	3.205284	4.329295	9.926034
N	3.385577	5.245275	12.092830
N	1.988707	1.009009	7.963821
C	3.671225	5.473973	9.402021
H	3.757157	5.494903	8.322692
C	4.009111	6.538486	10.190951
H	4.384288	7.462102	9.774481
C	3.839739	6.369652	11.570699
C	3.080658	4.253943	11.267981
C	2.587087	2.974929	11.749379
C	2.424692	2.706436	13.101018
H	2.648853	3.463514	13.843461
C	1.976361	1.454417	13.500491
C	1.707230	0.490168	12.530970
H	1.367130	-0.497275	12.816635
C	1.874965	0.780996	11.178813
H	1.658572	-0.007358	10.466519
C	2.309652	2.028282	10.741670
C	0.701816	0.641875	8.022389
H	0.055217	1.265810	8.624065
C	0.222748	-0.468801	7.356255
H	-0.827092	-0.719910	7.431672
C	1.099950	-1.236263	6.607532
H	0.752766	-2.115280	6.078163
C	2.429900	-0.854148	6.548397
H	3.155673	-1.416814	5.976039
C	2.836568	0.275252	7.231305
H	3.860506	0.620224	7.200635
O	1.837408	1.260662	14.835616
C	1.388777	-0.002768	15.274787
H	1.344982	0.050953	16.361017
H	0.391493	-0.231736	14.885425
H	2.081128	-0.798571	14.981648
O	4.152358	7.385134	12.358275
C	3.977958	7.218745	13.765019
H	2.933056	7.016841	14.001969
H	4.597106	6.401525	14.135770

H	4.290994	8.161642	14.206290

Comp 4

Pt	2.659048	2.721488	8.895933
Cl	3.148447	3.675327	6.722615
N	3.209648	4.362803	9.939869
N	3.372473	5.265614	12.114016
N	2.049979	1.031055	7.956926
C	3.671679	5.513831	9.426454
H	3.764171	5.542167	8.347772
C	3.998949	6.575052	10.224386
H	4.371288	7.503607	9.816427
C	3.823617	6.395678	11.601983
C	3.077780	4.278029	11.280591
C	2.589313	2.993003	11.750826
C	2.416220	2.716828	13.099673
H	2.627792	3.472130	13.847564
C	1.973050	1.459956	13.489001
C	1.720196	0.498380	12.512419
H	1.383911	-0.492662	12.790176
C	1.898749	0.796723	11.163338
H	1.694705	0.010689	10.444926
C	2.328206	2.049388	10.735638
C	0.766029	0.636734	8.000293
H	0.099314	1.248665	8.592405
C	0.307172	-0.474672	7.340421
H	-0.736087	-0.755340	7.398733
C	1.201671	-1.242709	6.591938
C	2.532874	-0.833740	6.543206
H	3.283069	-1.371563	5.981884
C	2.903590	0.303252	7.230245
H	3.925022	0.656873	7.200217
O	1.822358	1.259015	14.822077
C	1.375206	-0.008355	15.250781
H	1.318369	0.040624	16.336654
H	0.383745	-0.240971	14.848861
H	2.075011	-0.799524	14.962734
O	4.127618	7.407345	12.398302
C	3.949994	7.228997	13.803024
H	2.905751	7.018401	14.035388
H	4.573213	6.412809	14.169378
H	4.255728	8.170398	14.252599
O	0.709379	-2.315136	5.976444
C	1.593446	-3.117436	5.206257
H	2.386674	-3.534539	5.831438
H	0.986850	-3.923813	4.801908
H	2.029622	-2.541346	4.386755

Comp 5

Pt	2.616211	2.680915	8.903527
Cl	3.087015	3.601832	6.717647
N	3.203098	4.317467	9.929547
N	3.387557	5.241264	12.092180
N	1.956571	1.010445	7.971523
C	3.677381	5.456656	9.400362
H	3.764498	5.472648	8.321153
C	4.021676	6.521947	10.184991
H	4.403673	7.441025	9.764763
C	3.849779	6.360494	11.565482
C	3.077062	4.248619	11.271771
C	2.577236	2.973868	11.757973

C	2.414908	2.710272	13.110186
H	2.640960	3.469409	13.849894
C	1.965474	1.459776	13.514258
C	1.696924	0.492022	12.548380
H	1.358454	-0.494928	12.837360
C	1.864832	0.778353	11.195095
H	1.652711	-0.015863	10.487898
C	2.297861	2.024280	10.753901
C	0.681379	0.613155	8.055128
H	0.032805	1.198123	8.693294
C	0.234890	-0.488120	7.356354
H	-0.797179	-0.803983	7.420120
C	1.161917	-1.162831	6.582542
H	0.883527	-2.043278	6.012412
C	2.776151	0.299124	7.184183
H	3.798165	0.649245	7.119191
O	1.826673	1.271104	14.849481
C	1.379257	0.008791	15.293861
H	1.335430	0.067068	16.379803
H	0.382244	-0.222549	14.905334
H	2.072601	-0.787261	15.003947
O	4.168084	7.376927	12.348498
C	3.992479	7.217883	13.756229
H	2.946323	7.023383	13.993657
H	4.606733	6.398576	14.130390
H	4.311248	8.160859	14.193097
N	2.430852	-0.770610	6.498844

Comp 6

Pt	-2.512757	-0.234549	-0.038708
Cl	-4.857010	-0.812623	-0.196700
N	-1.834174	-2.071925	-0.530918
N	0.127905	-3.326047	-0.930256
N	-3.077218	1.652918	0.424898
C	-2.586717	-3.136070	-0.809482
H	-3.657768	-2.986889	-0.744598
C	-2.009803	-4.339419	-1.159926
H	-2.618791	-5.203251	-1.386195
C	-0.626927	-4.380944	-1.208714
H	-0.104447	-5.293093	-1.480804
C	-0.483810	-2.200141	-0.597487
C	0.243110	-0.989791	-0.259717
C	1.632735	-0.935405	-0.264854
H	2.200702	-1.814478	-0.545751
C	2.275924	0.238947	0.099219
C	1.496108	1.339764	0.463450
H	1.989853	2.256890	0.765984
C	0.111017	1.281398	0.441042
H	-0.439967	2.166900	0.736778
C	-0.562975	0.115511	0.073421
C	-2.848536	2.661535	-0.426239
H	-2.316123	2.409159	-1.332998
C	-3.264743	3.951983	-0.165360
H	-3.059464	4.731102	-0.887579
C	-3.934631	4.217923	1.017593
H	-4.268959	5.221694	1.250167
C	-4.169751	3.172883	1.895622
H	-4.690436	3.326051	2.831698
C	-3.734191	1.905035	1.564441
H	-3.908346	1.057250	2.212106
N	3.685660	0.324413	0.109932
C	4.445904	-0.729644	0.648468

C	4.013817	-1.402054	1.793279
H	3.089807	-1.100503	2.272088
C	4.756779	-2.448783	2.314601
H	4.404010	-2.956993	3.205198
C	5.948341	-2.837681	1.717115
H	6.529519	-3.653503	2.130342
C	6.383664	-2.167774	0.581443
H	7.306908	-2.464114	0.095904
C	5.639744	-1.129546	0.044873
H	5.982092	-0.622410	-0.849220
C	4.315550	1.451531	-0.448234
C	5.455466	1.998545	0.144673
H	5.858084	1.547349	1.043694
C	6.069150	3.110122	-0.408999
H	6.952201	3.520508	0.068230
C	5.554118	3.708044	-1.551869
H	6.033519	4.581119	-1.978491
C	4.416266	3.171865	-2.139373
H	4.004172	3.621345	-3.036081
C	3.804317	2.051420	-1.600667
H	2.922876	1.634224	-2.072870

Comp 7

Pt	-2.166059	-0.932125	-0.095759
Cl	-4.372605	-1.912908	-0.269725
N	-1.171599	-2.641920	-0.497321
N	0.985664	-3.552554	-0.814731
N	-3.060707	0.843871	0.294594
C	-1.722360	-3.833127	-0.729610
H	-2.804077	-3.869996	-0.682347
C	-0.938974	-4.932725	-1.014388
H	-1.384558	-5.899276	-1.202949
C	0.430694	-4.734697	-1.048702
H	1.108448	-5.553353	-1.271163
C	0.181708	-2.536372	-0.542973
C	0.681276	-1.204253	-0.254048
C	2.040189	-0.908642	-0.246365
H	2.758189	-1.686173	-0.479461
C	2.462388	0.374296	0.070612
C	1.497107	1.337977	0.373446
H	1.819133	2.339445	0.637969
C	0.143818	1.038054	0.339619
H	-0.558856	1.825062	0.588486
C	-0.310668	-0.242912	0.020328
C	-3.008584	1.856915	-0.575455
H	-2.427094	1.687829	-1.471831
C	-3.646831	3.062163	-0.370794
H	-3.560387	3.832749	-1.122959
C	-4.379948	3.241638	0.801003
C	-4.434281	2.182197	1.709170
H	-4.995839	2.281238	2.628591
C	-3.776351	1.014575	1.419177
H	-3.811573	0.171104	2.094546
N	3.836721	0.701864	0.097385
C	4.747903	-0.169405	0.721401
C	4.398701	-0.833980	1.898662
H	3.421409	-0.666815	2.335616
C	5.290997	-1.703189	2.505035
H	5.000231	-2.208309	3.419474
C	6.550380	-1.918083	1.961284
H	7.247742	-2.594816	2.440671
C	6.902881	-1.255061	0.793226

H	7.878575	-1.418131	0.348933
C	6.011687	-0.395142	0.172294
H	6.292294	0.106707	-0.745968
C	4.278625	1.886037	-0.518524
C	5.298557	2.650756	0.052191
H	5.754450	2.325339	0.979594
C	5.726147	3.817909	-0.558973
H	6.518071	4.397779	-0.097893
C	5.139680	4.255898	-1.739307
H	5.473125	5.172466	-2.211341
C	4.119751	3.502886	-2.305102
H	3.654638	3.825574	-3.230054
C	3.695260	2.326570	-1.708292
H	2.905635	1.740838	-2.163671
O	-5.038604	4.350717	1.126363
C	-5.009812	5.445115	0.220832
H	-5.449144	5.168014	-0.740435
H	-5.606919	6.227796	0.681786
H	-3.987969	5.803175	0.074036

Comp 8

Pt	2.554710	0.041914	0.018536
Cl	4.875367	0.722518	-0.103054
N	1.803332	1.887843	-0.326039
N	-0.202480	3.098812	-0.603382
N	3.188760	-1.853656	0.342593
C	2.510954	3.011724	-0.520920
H	3.587353	2.902129	-0.475905
C	1.899493	4.210832	-0.761709
H	2.463715	5.118701	-0.918739
C	0.499407	4.200421	-0.796013
C	0.457087	1.972926	-0.372375
C	-0.227283	0.714472	-0.133942
C	-1.613706	0.611789	-0.138393
H	-2.214846	1.490414	-0.341111
C	-2.213616	-0.610609	0.127815
C	-1.394400	-1.710987	0.391476
H	-1.854465	-2.667521	0.615033
C	-0.012008	-1.602145	0.369765
H	0.571415	-2.490041	0.585384
C	0.619615	-0.385921	0.103132
C	3.014648	-2.801068	-0.588207
H	2.487661	-2.499026	-1.482958
C	3.477810	-4.091007	-0.420208
H	3.315288	-4.818684	-1.204371
C	4.139382	-4.422378	0.750900
H	4.509914	-5.427524	0.911510
C	4.319048	-3.440495	1.711051
H	4.831225	-3.645856	2.641834
C	3.837691	-2.168565	1.470907
H	3.967697	-1.367746	2.185360
N	-3.620644	-0.741313	0.142324
C	-4.401340	0.225098	0.801980
C	-3.965993	0.785687	2.004469
H	-3.024683	0.463101	2.433215
C	-4.727715	1.748423	2.646593
H	-4.372095	2.169415	3.580526
C	-5.941307	2.162331	2.113781
H	-6.537373	2.911502	2.621279
C	-6.379856	1.603375	0.920652
H	-7.320713	1.921144	0.484993
C	-5.617823	0.650500	0.264387

H	-5.963540	0.230414	-0.672520
C	-4.223533	-1.825774	-0.519024
C	-5.346368	-2.456807	0.021146
H	-5.756763	-2.104580	0.959925
C	-5.933447	-3.526372	-0.634524
H	-6.803411	-4.003220	-0.196637
C	-5.408455	-3.999457	-1.830126
H	-5.866978	-4.840141	-2.337157
C	-4.287189	-3.380366	-2.365702
H	-3.867044	-3.731751	-3.301641
C	-3.701800	-2.300612	-1.724109
H	-2.832993	-1.818331	-2.156013
O	-0.119244	5.345333	-1.030375
C	-1.546291	5.339564	-1.065810
H	-1.908828	4.684426	-1.858345
H	-1.953839	5.009861	-0.109876
H	-1.832140	6.369286	-1.265106

Comp 9

Pt	-2.194682	-0.875621	-0.017273
Cl	-4.289775	-2.076982	-0.148083
N	-1.029579	-2.501688	-0.315079
N	1.206487	-3.214476	-0.560282
N	-3.261607	0.823801	0.265155
C	-1.452702	-3.763146	-0.491957
H	-2.525324	-3.907716	-0.454088
C	-0.575599	-4.789919	-0.707532
H	-0.910296	-5.807222	-0.850087
C	0.783314	-4.452587	-0.736583
C	0.299705	-2.270379	-0.352737
C	0.668658	-0.883021	-0.132754
C	1.992925	-0.459492	-0.127825
H	2.785110	-1.176231	-0.310014
C	2.287804	0.872870	0.122280
C	1.231488	1.755161	0.361908
H	1.453476	2.795579	0.573930
C	-0.086955	1.326385	0.330788
H	-0.864424	2.055623	0.528329
C	-0.414779	-0.007285	0.078010
C	-3.293738	1.790242	-0.657221
H	-2.689500	1.628397	-1.539824
C	-4.042301	2.940671	-0.520988
H	-4.019002	3.675406	-1.312650
C	-4.800777	3.113407	0.635484
C	-4.768577	2.102002	1.597721
H	-5.346886	2.196799	2.507174
C	-4.002662	0.986585	1.374287
H	-3.967381	0.179882	2.093195
N	3.625271	1.329454	0.144432
C	4.603783	0.580616	0.822758
C	4.300959	-0.048066	2.032244
H	3.307153	0.053677	2.451734
C	5.259987	-0.798823	2.692573
H	5.004376	-1.277200	3.631585
C	6.540410	-0.928375	2.171181
H	7.289751	-1.511961	2.692739
C	6.846658	-0.300432	0.971118
H	7.838717	-0.398164	0.544197
C	5.889772	0.440628	0.296894
H	6.136029	0.915528	-0.645250
C	3.965743	2.511823	-0.535630
C	4.907010	3.395993	-0.003444

H	5.379608	3.165779	0.943903
C	5.235894	4.560290	-0.677761
H	5.967857	5.233793	-0.245789
C	4.625933	4.876735	-1.884754
H	4.881615	5.791368	-2.406446
C	3.683234	4.004839	-2.412458
H	3.201291	4.232020	-3.356982
C	3.358461	2.830757	-1.751998
H	2.628916	2.152281	-2.177854
O	1.654558	-5.424759	-0.949128
C	3.040636	-5.085599	-0.980252
H	3.244754	-4.373608	-1.780321
H	3.354058	-4.657952	-0.027588
H	3.560870	-6.022134	-1.164788
O	-5.560461	4.173765	0.898398
C	-5.617632	5.219409	-0.061490
H	-6.018209	4.856290	-1.010934
H	-6.287890	5.967688	0.353852
H	-4.629958	5.659814	-0.218248

Comp 10

Pt	2.551205	0.035870	0.024254
Cl	4.873655	0.703412	-0.098450
N	1.802864	1.881014	-0.317375
N	-0.199277	3.094646	-0.605529
N	3.191428	-1.859124	0.330926
C	2.513861	3.003892	-0.507512
H	3.589785	2.893098	-0.456684
C	1.905459	4.203719	-0.751112
H	2.471954	5.110837	-0.904095
C	0.505432	4.195471	-0.794035
C	0.456909	1.968154	-0.370744
C	-0.230316	0.711244	-0.132262
C	-1.616621	0.610665	-0.139404
H	-2.215620	1.489148	-0.348750
C	-2.219389	-0.609452	0.132909
C	-1.402211	-1.708193	0.408670
H	-1.863526	-2.662008	0.640646
C	-0.019508	-1.601001	0.389809
H	0.559399	-2.488157	0.620368
C	0.614230	-0.388817	0.112729
C	2.960127	-2.831890	-0.558700
H	2.364902	-2.567017	-1.422207
C	3.462471	-4.101337	-0.368116
H	3.279171	-4.884141	-1.090978
C	4.199854	-4.321965	0.781170
H	4.618622	-5.298620	1.001383
C	3.930011	-2.167477	1.406358
H	4.119300	-1.361524	2.103531
N	-3.625727	-0.739201	0.142599
C	-4.410841	0.237401	0.782269
C	-3.984085	0.816435	1.978939
H	-3.045676	0.501058	2.419286
C	-4.751182	1.788019	2.601108
H	-4.402541	2.223474	3.531015
C	-5.961574	2.192200	2.053771
H	-6.561935	2.948175	2.545876
C	-6.391587	1.614661	0.866410
H	-7.329964	1.924468	0.419847
C	-5.624012	0.652882	0.229896
H	-5.962930	0.217786	-0.702650
C	-4.225943	-1.836232	-0.501122

C	-5.345648	-2.462290	0.050728
H	-5.755463	-2.096909	0.984738
C	-5.930433	-3.543581	-0.587639
H	-6.798082	-4.016595	-0.141137
C	-5.405881	-4.032894	-1.776859
H	-5.862582	-4.882614	-2.270287
C	-4.287753	-3.418314	-2.324094
H	-3.868499	-3.782287	-3.255602
C	-3.704869	-2.327055	-1.699936
H	-2.838861	-1.847927	-2.140943
O	-0.109872	5.340740	-1.032076
C	-1.536953	5.337728	-1.075361
H	-1.896159	4.683416	-1.870034
H	-1.950096	5.008674	-0.121652
H	-1.819564	6.368028	-1.276039
N	4.431273	-3.356472	1.667323

Comp 11

Pt	2.554728	-0.263747	0.066522
Cl	4.877002	0.406914	0.021245
N	1.822205	1.598875	-0.180508
N	-0.175059	2.833455	-0.405714
N	3.172839	-2.178007	0.280927
C	2.539044	2.710373	-0.309829
H	3.614655	2.588832	-0.263197
C	1.929510	3.939031	-0.494674
H	2.513560	4.841039	-0.600017
C	0.550277	3.931223	-0.536300
C	0.464235	1.690135	-0.229154
C	-0.224191	0.427684	-0.061550
C	-1.612716	0.334390	-0.071644
H	-2.209253	1.226143	-0.223836
C	-2.217761	-0.897838	0.125333
C	-1.401672	-2.015615	0.325240
H	-1.866148	-2.980879	0.495189
C	-0.019587	-1.913864	0.310445
H	0.558677	-2.815406	0.476607
C	0.617720	-0.687458	0.113791
C	3.000663	-3.063891	-0.709129
H	2.482433	-2.703688	-1.587303
C	3.456186	-4.363981	-0.618018
H	3.296592	-5.040542	-1.447192
C	4.106378	-4.770954	0.535507
H	4.470581	-5.786151	0.635905
C	4.283041	-3.852237	1.556784
H	4.786496	-4.118368	2.476802
C	3.810857	-2.565009	1.392838
H	3.939570	-1.810853	2.156485
N	-3.623172	-1.024955	0.136828
C	-4.402839	-0.085892	0.838041
C	-3.971243	0.415727	2.067191
H	-3.032790	0.070796	2.484788
C	-4.733670	1.349196	2.750414
H	-4.381203	1.725843	3.704207
C	-5.943989	1.789882	2.232166
H	-6.540385	2.516302	2.771320
C	-6.378848	1.288630	1.012426
H	-7.317040	1.628874	0.588278
C	-5.615649	0.366199	0.315305
H	-5.957517	-0.009086	-0.641850
C	-4.230622	-2.085148	-0.560131
C	-5.344430	-2.740786	-0.031479

H	-5.744014	-2.427258	0.925516
C	-5.936429	-3.785280	-0.722301
H	-6.799495	-4.282413	-0.293481
C	-5.424823	-4.207765	-1.942376
H	-5.887192	-5.028939	-2.477133
C	-4.312678	-3.563473	-2.467115
H	-3.904038	-3.874991	-3.422044
C	-3.722886	-2.508055	-1.790014
H	-2.862410	-2.004045	-2.213850
C	-0.251739	5.201900	-0.738436
F	0.540448	6.268365	-0.862065
F	-1.002447	5.123324	-1.839404
F	-1.070154	5.420669	0.293050

Comp 12

Pt	2.588180	2.733349	8.899064
Cl	3.002491	3.617901	6.686889
N	3.099270	4.425607	9.875287
N	3.281551	5.396701	12.021159
N	2.034398	0.994571	8.022071
C	3.506017	5.562718	9.311432
H	3.570986	5.556691	8.230052
C	3.816841	6.663693	10.082518
H	4.146976	7.586580	9.626956
C	3.683913	6.526296	11.453667
H	3.908724	7.351845	12.122218
C	2.999449	4.374219	11.228627
C	2.563277	3.088218	11.741544
C	2.419079	2.839559	13.101527
H	2.611656	3.643446	13.802963
C	2.011360	1.587860	13.548755
C	1.765151	0.605444	12.582672
H	1.474954	-0.389892	12.903126
C	1.910156	0.856661	11.226373
H	1.718761	0.046172	10.532377
C	2.306704	2.110756	10.760066
C	0.757826	0.590209	8.043742
H	0.067204	1.219595	8.588224
C	0.342117	-0.563908	7.409889
H	-0.701832	-0.845296	7.452639
C	1.274144	-1.334984	6.734819
H	0.977032	-2.247344	6.232120
C	2.593492	-0.913812	6.714368
H	3.359920	-1.478041	6.199552
C	2.935962	0.257114	7.361395
H	3.949800	0.632433	7.359636
C	1.850579	1.302999	14.988096
C	0.843870	0.448509	15.443701
C	2.700421	1.881155	15.934035
C	0.692076	0.181602	16.795629
H	0.156353	0.004487	14.732355
C	2.548755	1.615921	17.286131
H	3.504193	2.530130	15.604535
C	1.543680	0.764321	17.724102
H	-0.101911	-0.478908	17.125930
H	3.225397	2.070887	18.000927
H	1.425120	0.556193	18.781274

Comp 13

Pt	2.643203	2.754746	8.910045
Cl	3.079894	3.651346	6.705169

N	3.114697	4.453223	9.894409
N	3.237394	5.429190	12.042710
N	2.110890	1.009577	8.025588
C	3.509103	5.598110	9.337541
H	3.593430	5.592607	8.257483
C	3.783206	6.705628	10.113226
H	4.102811	7.634908	9.663128
C	3.627060	6.566504	11.481763
H	3.821768	7.397090	12.153560
C	2.991137	4.400684	11.245842
C	2.572588	3.106101	11.751575
C	2.413917	2.853889	13.109267
H	2.578848	3.661944	13.812888
C	2.027031	1.593572	13.550621
C	1.818354	0.605964	12.580780
H	1.546614	-0.395983	12.896863
C	1.977149	0.860869	11.226779
H	1.815349	0.046711	10.529605
C	2.350683	2.124246	10.765762
C	0.841688	0.569771	8.064060
H	0.143190	1.175806	8.624789
C	0.435235	-0.579695	7.436126
H	-0.597648	-0.897300	7.488452
C	1.369744	-1.338527	6.727869
C	2.685979	-0.882478	6.685825
H	3.464513	-1.411005	6.155285
C	3.003280	0.290089	7.338175
H	4.011589	0.679804	7.311541
C	1.849219	1.305348	14.987281
C	0.858215	0.424127	15.426280
C	2.665975	1.907107	15.947640
C	0.689796	0.154105	16.775605
H	0.195576	-0.038876	14.703551
C	2.497424	1.639060	17.297157
H	3.457353	2.577793	15.631968
C	1.508475	0.760540	17.718393
H	-0.091619	-0.527649	17.092486
H	3.148428	2.113141	18.023264
H	1.376829	0.550180	18.773577
O	0.927945	-2.447903	6.141613
C	1.853358	-3.240716	5.410685
H	2.652386	-3.605931	6.060289
H	1.283845	-4.082627	5.025438
H	2.279077	-2.675302	4.578390

Comp 14

Pt	2.590396	-0.203991	-0.036669
Cl	4.941839	-0.736546	-0.190356
N	1.946484	-2.065487	-0.483111
N	0.006071	-3.377909	-0.789544
N	3.120128	1.692249	0.434989
C	2.717859	-3.121541	-0.741097
H	3.786282	-2.946134	-0.705039
C	2.161284	-4.349634	-1.033586
H	2.785136	-5.206990	-1.243361
C	0.779036	-4.425974	-1.044093
H	0.272306	-5.360439	-1.265029
C	0.599294	-2.226838	-0.517659
C	-0.148915	-1.014943	-0.233538
C	-1.538953	-0.981115	-0.248984
H	-2.098351	-1.879404	-0.482554
C	-2.190267	0.208807	0.028891

C	-1.438704	1.350612	0.303591
H	-1.951880	2.278669	0.530848
C	-0.052585	1.309934	0.291783
H	0.486887	2.226495	0.499911
C	0.636417	0.123653	0.032411
C	2.969273	2.154221	1.683061
H	2.516492	1.474673	2.392241
C	3.366600	3.425047	2.048403
H	3.227006	3.750374	3.070895
C	3.934740	4.253515	1.094522
H	4.252601	5.256508	1.352130
C	4.089777	3.772105	-0.194941
H	4.529792	4.377737	-0.976174
C	3.677677	2.486885	-0.487177
H	3.789877	2.064284	-1.476036
C	-6.325891	2.569392	-2.051331
C	-4.971738	2.769313	-2.338615
C	-3.980663	2.050800	-1.691396
C	-4.376558	1.119568	-0.737160
C	-5.738409	0.897002	-0.444122
C	-6.715278	1.633595	-1.109304
H	-7.074667	3.151343	-2.575858
H	-4.688853	3.502025	-3.085969
H	-2.935116	2.209077	-1.925411
H	-7.766104	1.474090	-0.893805
C	-4.443144	-0.499081	0.821054
C	-4.124841	-1.467262	1.767308
C	-5.170687	-2.082315	2.434628
C	-6.503083	-1.746127	2.173884
C	-6.814347	-0.775183	1.238430
C	-5.781080	-0.140160	0.553968
H	-3.096358	-1.732634	1.978846
H	-4.948745	-2.841596	3.176000
H	-7.296440	-2.250306	2.713183
H	-7.847795	-0.510641	1.042753
N	-3.601991	0.269685	0.034107

Comp 15

Pt	2.279544	-0.835641	-0.124767
Cl	4.528788	-1.708787	-0.265642
N	1.372967	-2.633351	-0.282666
N	-0.737175	-3.696133	-0.312756
N	3.082544	1.014511	0.069977
C	1.982944	-3.812519	-0.403140
H	3.065493	-3.783457	-0.431078
C	1.254492	-4.981476	-0.483516
H	1.747637	-5.938309	-0.581427
C	-0.124132	-4.866999	-0.430507
H	-0.760731	-5.744861	-0.484509
C	0.016528	-2.610671	-0.243746
C	-0.548933	-1.278005	-0.128414
C	-1.921170	-1.053925	-0.115411
H	-2.606785	-1.890500	-0.183978
C	-2.393888	0.243995	-0.024254
C	-1.485799	1.299904	0.036167
H	-1.860995	2.314927	0.110789
C	-0.119257	1.065220	0.003852
H	0.547158	1.918963	0.041124
C	0.393124	-0.232028	-0.066735
C	2.980922	1.698080	1.214102
H	2.412105	1.226443	2.004233
C	3.555154	2.936562	1.407824

H	3.431796	3.424802	2.363521
C	4.273698	3.513002	0.361645
C	4.380067	2.797444	-0.832952
H	4.932795	3.209093	-1.666918
C	3.784771	1.566257	-0.934162
H	3.862325	0.981132	-1.839856
C	-6.300789	2.641725	-2.470400
C	-4.948866	2.591754	-2.825982
C	-4.023940	1.902948	-2.059555
C	-4.484719	1.260135	-0.915614
C	-5.846389	1.292054	-0.547511
C	-6.755687	1.992670	-1.336039
H	-6.996652	3.191382	-3.093400
H	-4.615442	3.101629	-3.722812
H	-2.979858	1.864922	-2.345413
H	-7.805700	2.026372	-1.066736
C	-4.671662	0.038471	0.960911
C	-4.426356	-0.740372	2.086534
C	-5.503018	-1.050314	2.900187
C	-6.794193	-0.598344	2.608112
C	-7.031618	0.182674	1.490732
C	-5.966023	0.509879	0.655857
H	-3.429357	-1.092499	2.321552
H	-5.338874	-1.657042	3.783577
H	-7.613751	-0.862066	3.266332
H	-8.032576	0.536992	1.269816
N	-3.784308	0.499331	0.003956
O	4.871892	4.699858	0.410702
C	4.790010	5.449864	1.614846
H	5.247956	4.906320	2.444622
H	5.343150	6.367422	1.431319
H	3.751537	5.690475	1.854849

Comp 17

Pt	2.620531	2.713131	8.889413
Cl	3.024932	3.653776	6.695617
N	3.193173	4.347606	9.914159
N	1.985619	1.027859	7.960688
N	3.893429	6.501478	11.501976
C	3.623738	5.487470	9.373096
H	3.678645	5.518523	8.292628
C	3.971839	6.557425	10.175426
H	4.321080	7.480681	9.727658
C	3.466958	5.365850	12.027592
H	3.403092	5.317478	13.108660
C	3.106292	4.257896	11.260424
C	2.641811	2.973226	11.749872
C	2.509123	2.672129	13.100007
H	2.732681	3.397294	13.874016
C	2.083629	1.407835	13.488045
C	1.802947	0.455775	12.511562
H	1.479573	-0.539688	12.787945
C	1.938667	0.773853	11.162453
H	1.715195	-0.003274	10.440277
C	2.350280	2.032070	10.737216
C	0.699600	0.658149	8.020167
H	0.050866	1.281998	8.619667
C	0.224183	-0.455625	7.356855
H	-0.824944	-0.709474	7.432146
C	1.104419	-1.222824	6.611536
H	0.760010	-2.104512	6.084777
C	2.433484	-0.837657	6.551931

H	3.160922	-1.400294	5.981784
C	2.836605	0.295104	7.231035
H	3.859415	0.643542	7.199768
O	1.978328	1.195066	14.822283
C	1.557135	-0.080546	15.254927
H	1.539315	-0.041620	16.342435
H	0.553876	-0.317448	14.886587
H	2.253043	-0.862202	14.933917

Comp 18

Pt	-2.509903	-0.230101	-0.037662
Cl	-4.862167	-0.773374	-0.184623
N	-1.837245	-2.074321	-0.515817
N	-3.061365	1.664474	0.414264
N	-2.167355	-4.328512	-1.117902
C	-2.606509	-3.131924	-0.784170
H	-3.674739	-2.961734	-0.715828
C	-0.843023	-4.475943	-1.190164
H	-0.477663	-5.459989	-1.466667
C	0.037485	-3.448282	-0.931147
H	1.105164	-3.603931	-0.996687
C	-0.489183	-2.210798	-0.582309
C	0.246120	-1.005959	-0.257453
C	1.637989	-0.940804	-0.261894
H	2.233349	-1.803381	-0.537452
C	2.280018	0.234944	0.098163
C	1.497800	1.335733	0.457696
H	1.989075	2.254818	0.757790
C	0.114130	1.273165	0.433182
H	-0.439045	2.158646	0.724234
C	-0.560098	0.105424	0.070586
C	-2.837891	2.664457	-0.448199
H	-2.317545	2.401815	-1.359065
C	-3.245076	3.959062	-0.193683
H	-3.044814	4.730959	-0.925001
C	-3.900126	4.238197	0.994532
H	-4.227260	5.245448	1.222229
C	-4.130105	3.201852	1.884140
H	-4.639542	3.365422	2.824628
C	-3.704308	1.929173	1.558871
H	-3.875205	1.087676	2.215498
N	3.688218	0.320458	0.109596
C	4.450528	-0.742734	0.629034
C	4.030913	-1.422058	1.774281
H	3.116092	-1.118684	2.269494
C	4.775698	-2.477083	2.276051
H	4.433784	-2.990561	3.167825
C	5.956684	-2.866589	1.658085
H	6.539750	-3.688407	2.056468
C	6.380067	-2.188881	0.522592
H	7.295553	-2.484929	0.022496
C	5.633775	-1.142378	0.005367
H	5.966548	-0.627871	-0.888180
C	4.319678	1.454361	-0.434704
C	5.458592	1.992337	0.167721
H	5.858124	1.529830	1.062385
C	6.075080	3.109500	-0.371374
H	6.957476	3.513205	0.112628
C	5.563347	3.721285	-1.508365
H	6.044739	4.598834	-1.923380
C	4.426527	3.193591	-2.105295

H	4.017380	3.654185	-2.997657
C	3.812013	2.067429	-1.581438
H	2.931532	1.656739	-2.061154

Comp 19

Pt	2.580083	2.735530	8.907033
Cl	2.988788	3.606771	6.688690
N	3.082113	4.425853	9.877530
N	2.033263	0.991634	8.032583
N	3.699769	6.651873	11.396848
C	3.481073	5.559874	9.301318
H	3.545473	5.556137	8.220944
C	3.788222	6.666450	10.069717
H	4.112492	7.584747	9.593959
C	3.304233	5.521993	11.957323
H	3.232280	5.508925	13.038886
C	2.985239	4.377659	11.225272
C	2.556562	3.096004	11.752438
C	2.410540	2.830465	13.111004
H	2.592410	3.610069	13.842336
C	2.006012	1.574495	13.550821
C	1.760279	0.596884	12.581947
H	1.471373	-0.400387	12.896979
C	1.906237	0.859118	11.228067
H	1.716505	0.053765	10.527771
C	2.300742	2.115463	10.768865
C	0.754785	0.593068	8.037160
H	0.058005	1.229678	8.565196
C	0.344677	-0.564551	7.406149
H	-0.700965	-0.841395	7.434135
C	1.284471	-1.344923	6.752900
H	0.991751	-2.260214	6.252978
C	2.605812	-0.929506	6.750433
H	3.378034	-1.501198	6.252845
C	2.942664	0.245442	7.393011
H	3.958089	0.616383	7.404679
C	1.847637	1.283276	14.989136
C	0.829868	0.440861	15.442317
C	2.710283	1.841567	15.935232
C	0.679122	0.167282	16.792970
H	0.133593	0.012196	14.730086
C	2.559612	1.569607	17.286180
H	3.524412	2.478357	15.607107
C	1.542997	0.730841	17.721985
H	-0.123451	-0.483369	17.121961
H	3.246297	2.008507	18.001392
H	1.425216	0.517353	18.778150

Comp 20

Pt	2.586541	-0.199077	-0.036777
Cl	4.943695	-0.706763	-0.183314
N	1.954899	-2.057780	-0.481213
N	0.881416	-4.538220	-1.064790
N	3.106637	1.701566	0.434867
C	2.742426	-3.103014	-0.733676
H	3.809247	-2.924471	-0.696766
C	2.195434	-4.338464	-1.025116
H	2.842240	-5.183684	-1.230093
C	0.109866	-3.494277	-0.813854
H	-0.961520	-3.656582	-0.845963
C	0.614263	-2.228047	-0.518091

C	-0.151387	-1.027313	-0.238425
C	-1.542944	-0.980922	-0.251627
H	-2.133938	-1.858541	-0.485987
C	-2.192263	0.210189	0.030371
C	-1.441402	1.350114	0.306101
H	-1.952251	2.278616	0.535898
C	-0.055615	1.303278	0.291399
H	0.487650	2.217412	0.499819
C	0.631070	0.117212	0.030304
C	2.960224	2.159714	1.684809
H	2.516752	1.475711	2.395626
C	3.351044	3.432549	2.049993
H	3.215839	3.755019	3.073962
C	3.907215	4.266601	1.093935
H	4.219669	5.271314	1.351427
C	4.057554	3.788826	-0.197453
H	4.488491	4.399014	-0.980170
C	3.652967	2.501230	-0.489535
H	3.762365	2.081094	-1.479785
C	-6.332951	2.556486	-2.055041
C	-4.979145	2.761995	-2.339876
C	-3.986282	2.047518	-1.690894
C	-4.380342	1.114844	-0.737465
C	-5.741609	0.886602	-0.446791
C	-6.720308	1.619152	-1.113745
H	-7.083112	3.135565	-2.580735
H	-4.697923	3.496111	-3.086453
H	-2.940917	2.210436	-1.922562
H	-7.770826	1.455605	-0.899888
C	-4.443237	-0.503052	0.822432
C	-4.122719	-1.467552	1.771656
C	-5.167349	-2.086843	2.437109
C	-6.500540	-1.757727	2.171885
C	-6.813935	-0.789251	1.234539
C	-5.781984	-0.150233	0.551864
H	-3.093421	-1.725599	1.988548
H	-4.943714	-2.843157	3.180980
H	-7.292915	-2.264912	2.709760
H	-7.848088	-0.529623	1.036134
N	-3.603663	0.268143	0.035756

Comp 21

Pt	2.473747	-0.152867	-0.284758
Cl	4.754983	0.383870	-0.898372
N	1.692552	1.671631	-0.652377
N	3.144810	-2.001702	0.199066
C	2.412248	2.703324	-1.154045
H	3.428963	2.453924	-1.434234
C	0.732399	4.191392	-0.866083
C	-0.092786	3.192377	-0.284017
C	0.410135	1.859361	-0.300523
C	-0.283293	0.619451	0.014855
C	-1.668484	0.481064	0.099478
H	-2.342864	1.305201	-0.082028
C	-2.236667	-0.758944	0.355698
C	-1.410923	-1.868040	0.515091
H	-1.829507	-2.846932	0.711484
C	-0.033219	-1.732389	0.383591
H	0.569355	-2.628992	0.471547
C	0.570465	-0.507943	0.118015
C	3.683998	-2.791986	-0.738284
H	3.715012	-2.388290	-1.740499

C	4.178097	-4.047498	-0.444009
H	4.597019	-4.651281	-1.238234
C	4.131746	-4.501395	0.863756
C	3.584999	-3.676548	1.833202
H	3.529384	-3.980771	2.870123
C	3.098401	-2.437964	1.464690
H	2.655375	-1.764198	2.185206
C	-1.309487	3.593766	0.311263
C	-1.716989	4.899522	0.251320
H	-2.644152	5.193643	0.728318
C	-0.935107	5.865131	-0.406732
H	-1.279838	6.891375	-0.457192
C	0.274139	5.520166	-0.945762
H	0.919581	6.251382	-1.416972
H	-1.902481	2.883488	0.866620
N	1.978578	3.912483	-1.327093
O	-3.590239	-0.792699	0.415972
C	-4.208595	-2.041829	0.638894
H	-5.280415	-1.853180	0.643318
H	-3.971226	-2.753740	-0.158061
H	-3.914539	-2.468170	1.603241
H	4.516549	-5.480163	1.123322

Comp 22

Pt	2.472535	-0.154000	-0.297177
Cl	4.748204	0.376967	-0.942528
N	1.691138	1.670596	-0.660984
N	3.145736	-2.004729	0.191205
C	2.408485	2.702332	-1.166086
H	3.423590	2.452246	-1.451801
C	0.730842	4.191224	-0.869243
C	-0.091618	3.192542	-0.283009
C	0.410712	1.859219	-0.302229
C	-0.281794	0.619745	0.016247
C	-1.666945	0.482002	0.104440
H	-2.341190	1.306890	-0.074234
C	-2.235028	-0.758055	0.359801
C	-1.409335	-1.867966	0.514580
H	-1.828017	-2.847089	0.709872
C	-0.031946	-1.732857	0.379809
H	0.570789	-2.629710	0.463513
C	0.572177	-0.508047	0.115625
C	3.712281	-2.793224	-0.727774
H	3.769528	-2.391650	-1.729933
C	4.209518	-4.047504	-0.442967
H	4.647662	-4.628491	-1.241459
C	4.136572	-4.516618	0.867259
C	3.555921	-3.687280	1.829385
H	3.484775	-4.012988	2.858635
C	3.076611	-2.458253	1.454354
H	2.615310	-1.796086	2.174239
C	-1.305129	3.594318	0.318509
C	-1.712617	4.900238	0.260753
H	-2.637353	5.194545	0.742346
C	-0.933774	5.865613	-0.401151
H	-1.278386	6.891983	-0.449846
C	0.272581	5.520150	-0.946371
H	0.915719	6.251181	-1.420947
H	-1.895792	2.884062	0.876507
N	1.974615	3.911869	-1.336662
O	-3.588729	-0.791435	0.423369
C	-4.206716	-2.040731	0.645674

H	-5.278579	-1.852252	0.651463
H	-3.970145	-2.751837	-0.152247
H	-3.911586	-2.468108	1.609266
O	4.580039	-5.701586	1.279025
C	5.178977	-6.567765	0.325123
H	6.067678	-6.108910	-0.114552
H	5.464256	-7.461847	0.873633
H	4.468612	-6.832308	-0.461835

Comp 23

Pt	2.570624	-0.050661	-0.020754
Cl	4.888673	0.571806	-0.304922
N	1.783619	1.766544	-0.411766
N	3.232292	-1.919810	0.403168
C	2.527652	2.833111	-0.789283
H	3.584240	2.627883	-0.915966
C	0.762868	4.248706	-0.748777
C	-0.097415	3.211777	-0.298460
C	0.456705	1.898996	-0.250483
C	-0.223215	0.633311	-0.030135
C	-1.605247	0.442074	-0.108395
H	-2.264311	1.241936	-0.411279
C	-2.163827	-0.799588	0.154294
C	-1.314066	-1.860969	0.472022
H	-1.739652	-2.832137	0.699290
C	0.060271	-1.695453	0.461006
H	0.678763	-2.559362	0.674307
C	0.650214	-0.460319	0.188077
C	3.152647	-2.893238	-0.512850
H	2.687614	-2.627993	-1.452627
C	3.634220	-4.165624	-0.276154
H	3.549048	-4.916930	-1.050143
C	4.215550	-4.449114	0.948819
H	4.599215	-5.439249	1.162926
C	4.297812	-3.439426	1.893349
H	4.744770	-3.607390	2.864337
C	3.801632	-2.188169	1.584775
H	3.853122	-1.367732	2.287225
N	-3.561092	-0.981737	0.102132
C	-4.414351	0.002068	0.637984
C	-4.089500	0.648366	1.832411
H	-3.179061	0.378929	2.354708
C	-4.923266	1.626701	2.349694
H	-4.654447	2.114741	3.279967
C	-6.100638	1.969874	1.698076
H	-6.753470	2.731167	2.108294
C	-6.430294	1.323525	0.514314
H	-7.341898	1.584329	-0.011783
C	-5.594895	0.354547	-0.017893
H	-5.855010	-0.135207	-0.948689
C	-4.095008	-2.132170	-0.508609
C	-5.211555	-2.770310	0.034736
H	-5.668374	-2.373400	0.933497
C	-5.733531	-3.903036	-0.567762
H	-6.600100	-4.385341	-0.129277
C	-5.147174	-4.430599	-1.710861
H	-5.554383	-5.320458	-2.176047
C	-4.032155	-3.802840	-2.249276
H	-3.566126	-4.196945	-3.145558
C	-3.512286	-2.660492	-1.661589
H	-2.648616	-2.171012	-2.095898
C	-1.403748	3.559942	0.112858

C	-1.851875	4.848338	-0.006672
H	-2.850797	5.100297	0.328589
C	-1.023067	5.849248	-0.542770
H	-1.399337	6.860461	-0.644752
C	0.266332	5.557843	-0.895342
H	0.943581	6.318019	-1.265118
H	-2.044525	2.825308	0.576536
N	2.075310	4.026211	-1.016773

Comp 24

Pt	-2.189913	-0.881176	-0.082104
Cl	-4.246757	-2.108247	-0.441954
N	-0.924750	-2.415795	-0.426239
N	-3.350592	0.737921	0.308012
C	-1.336481	-3.651274	-0.796884
H	-2.404796	-3.745615	-0.954108
C	0.746683	-4.527270	-0.681080
C	1.276515	-3.286450	-0.236498
C	0.382265	-2.176310	-0.230513
C	0.681984	-0.769350	-0.022132
C	1.958538	-0.204336	-0.086797
H	2.819516	-0.795841	-0.361027
C	2.144797	1.148986	0.148582
C	1.029119	1.939557	0.430370
H	1.165987	2.995668	0.635546
C	-0.245088	1.399150	0.410041
H	-1.083449	2.060435	0.594797
C	-0.464334	0.043395	0.159237
C	-3.562458	1.675878	-0.619565
H	-3.052446	1.538465	-1.563792
C	-4.377501	2.769476	-0.415469
H	-4.501221	3.484843	-1.215430
C	-5.013312	2.910675	0.816855
C	-4.793721	1.927767	1.784247
H	-5.272346	1.999226	2.751873
C	-3.970992	0.870162	1.492047
H	-3.788080	0.088781	2.216930
N	3.436859	1.714564	0.099959
C	4.517383	1.037569	0.695895
C	4.352230	0.374229	1.913753
H	3.387002	0.394401	2.405829
C	5.412379	-0.304785	2.492320
H	5.263734	-0.810773	3.439820
C	6.658457	-0.325663	1.879615
H	7.487093	-0.852489	2.337693
C	6.827617	0.338193	0.671974
H	7.791334	0.325417	0.175032
C	5.769220	1.007380	0.078786
H	5.909183	1.511086	-0.870133
C	3.638874	2.929003	-0.581903
C	4.525339	3.885829	-0.083636
H	5.062605	3.688140	0.836254
C	4.718154	5.080553	-0.757374
H	5.409524	5.811498	-0.352917
C	4.023558	5.353130	-1.928821
H	4.172685	6.291384	-2.449885
C	3.135295	4.407451	-2.422486
H	2.589677	4.600385	-3.339513
C	2.947057	3.203289	-1.762856
H	2.259830	2.466992	-2.162408
C	2.616076	-3.254469	0.212039
C	3.403736	-4.371907	0.134588

H	4.423631	-4.333720	0.497985
C	2.896477	-5.571502	-0.394509
H	3.538333	-6.442110	-0.462504
C	1.587240	-5.651939	-0.783592
H	1.155470	-6.575458	-1.149635
H	3.016865	-2.363145	0.670609
N	-0.568116	-4.678139	-0.985184
O	-5.819981	3.915137	1.148312
C	-6.068906	4.929536	0.185052
H	-6.544808	4.513242	-0.705951
H	-6.744854	5.633704	0.663399
H	-5.143546	5.440785	-0.091159