Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information for:

Synthesis, Structure, Photophysical and Electrochemical Properties of Ru(II) Complexes of Arylene-Vinylene Terpyridyl Conjugates

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1. Synthesis and Characterization

1a. Syntheses

Synthesis of 4'-(4-{2-[phenyl]-ethenyl}phenyl)-2,2':6',2''-terpyridine (L1): 4-(2,2':6',2''-Terpyridyl-4')-benzyl triphenylphosphonium bromide (1.0 g, 3.10 mmol) and potassium *tert*-butoxide (2.08 g, 18.60 mmol) were combined using a morter and pestle, and the yellow medium was aggregated until a light orange powder formed. To it benzaldehyde (0.47 mL, 4.65 mmol) was added and the combined mixture was grinded vigorously for about 30 min. After the mixture became sticky, 5 ml of dichloromethane was added and the mixture was continuously grinded for another 10 min. After completion of the reaction (monitored by TLC), the mixture was dispersed in 100 mL of dichloromethane and worked up with brine solution followed by water. The organic part was collected and dried over anhydrous $MgSO_4$, filtered and concentrated. The solid residue was stirred in distilled methanol for overnight at room temperature. The precipitated solid was isolated by vacuum filtration, washed with water (3×10 mL), methanol (5×10 mL) and diethyl ether (3×10 mL).The solid residue was further purified by column chromatography (ethyl acetate: hexanes, 4:1) on silica gel (60 - 120 mesh) to achieve analytically pure lemon yellow solid product. Yield: 0.71 g, (57%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ, 7.20 (d, *J* = 5.2 Hz, 2H), 7.26 (d, *J* = 6Hz,1H), 7.27-7.31(m, 1H) 7.36-7.42 (m, 4H) 7.57 (d, *J* =7.2 Hz, 2H), 7.67 (d, *J* = 8 Hz, 2H), 7.88-7.96 (m, 4H), 8.68 (d, *J* =8Hz, 2H), 8.76 (d, *J* = 4.8Hz, 2H), 8.79 (s, 2H) ; ^{13}C NMR {^{1}H} ($CDCl_3$, 100 MHz): δ 118.8, 121.6, 124.1, 126.9, 127.3, 127.8, 128.1, 128.2, 128.9, 129.8, 137.2, 137.4, 137.6, 138.4, 149.3, 149.7 156.2, 156.5. HRMS (ESI$^+$): $C_{29}H_{21}N_3$, Calculated value 412.4808 ([M+H]$^+$); experimental 412.1814 ([M+H]$^+$); FTIR (KBr, cm^{-1}): 2918 ($\bar{\upsilon}_{\text{C-H stretching}}$), 1585 ($\bar{\upsilon}_{\text{C=C stretching}}$); λ_{max}(ε): 333 nm (ε = 5.5×10^4 M^{-1}cm^{-1}), 287 nm (ε = 4.0×10^4 M^{-1}cm^{-1}); λ_{em}: 412 nm (λ_{ex}: 333 nm).

4'-(4-{2-[*p*-tolyl]-ethenyl} phenyl)-2, 2'-6', 2''-terpyridine (L2): L2 was prepared using a similar procedure as that for **L1** using 4-methylbenzaldehyde (0.56 mL, 4.65 mmol), 4-(2,2':6',2''-Terpyridyl-4')-benzyl triphenylphosphonium bromide (1.0 g, 3.10 mmol) and potassium *tert*-butoxide (2.08 g, 18.60 mmol). The pure product was isolated as lemon yellow solid product. Yield: 0.71 g (54%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.38 (s, 3H, methyl), 7.12 (d, *J* = 16 Hz, vinyl 1H), 7.14-7.21 (m, 3H), 7.35-7.37 (m, 2H), 7.45 (d, *J* = 8Hz, 2H), 7.63 (d, *J* = 8 Hz, 2H), 7.86 - 7.94 (m, 4H, Py), 8.68 (d, *J* = 8 Hz, 2H, Py), 8.76 (d, *J* = 4Hz, 2H, Py), 8.78 (s, 2H, Py) ; ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 21.6 (methyl), 118.8, 121.7, 124.1, 126.8, 127.2, 127.3, 127.8, 129.7, 129.8, 134.7, 137.1, 137.4, 138.1, 138.6, 149.4, 149.9, 156.2, 156.6; HRMS (ESI+): $C_{30}H_{23}N_3$, Calculated

value 426.1970 ([M+H]+); experimental 426.1973 ([M+H]+); FTIR (KBr, cm-1): 2923 ($\bar{\upsilon}_{\text{C-H stretching}}$), 1585 ($\bar{\upsilon}_{\text{C=C stretching}}$), 1566 ($\bar{\upsilon}_{\text{C=N stretching}}$); $\lambda_{max}(\varepsilon)$: 338 nm ($\varepsilon = 4.1\times10^4$ $M^{-1}cm^{-1}$), 288 nm ($\varepsilon = 3.2\times10^4$ $M^{-1}cm^{-1}$); λ_{em}: 423 nm (λ_{ex}: 338 nm).

4'-(4-{2-[1-Naphthyl]-ethenyl} phenyl)-2, 2'-6', 2''-terpyridine (L3): L3 was prepared analogously to **L1** using 1-naphthaldehyde (0.63 mL, 4.65 mmol), 4-(2,2':6',2''-terpyridyl-4')-benzyl triphenylphosphonium bromide (1.0 g, 3.10 mmol) and potassium *tert*-butoxide (2.08 g, 18.60 mmol). The pure product was isolated as pale yellow solid. Yield: 0.70 g (49%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.21 -7.26 (m, 2H), 7.36-7.39 (m, 2H), 7.50-7.58 (m, 2H), 7.74-7.76 (m, 2H, Py), 7.80-7.84 (m, 2H, Py), 7.88-7.92 (m, 3H), 7.98-8.02 (m, 3H), 8.28 (d, J = 8Hz,1H), 8.70 (d, J = 8 Hz, 2H, Py), 8.75-8.76 (m, 2H, Py), 8.8 (s, 2H, Py); $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 118.9, 121.7, 124.0, 125.9, 126.5, 126.9, 127.1, 127.6, 127.9, 128.5, 128.9, 129.2, 129.9, 131.3, 131.7, 134.0, 135.1, 137.2, 137.9, 138.7, 149.3, 150.0, 156.2, 156.5; HRMS (ESI^+): $C_{33}H_{24}N_3$, Calculated value 462.1970 ($[M+H]^+$); experimental 462.1967 ($[M+H]^+$); FTIR (KBr, cm^{-1}): 2926 ($\bar{\upsilon}_{\text{C-H stretching}}$), 1577 ($\bar{\upsilon}_{\text{C=C stretching}}$), 1566 ($\bar{\upsilon}_{\text{C=N stretching}}$); $\lambda_{max}(\varepsilon)$: 344 nm ($\varepsilon = 2.7\times10^4$ $M^{-1}cm^{-1}$), 284 nm ($\varepsilon = 3.3\times10^4$ $M^{-1}cm^{-1}$); λ_{em}: 433 nm (λ_{ex}: 344 nm).

4'-(4-{2-[9-Anthryl]-ethenyl} phenyl)-2, 2'-6', 2''-terpyridine (L4): L4 was prepared using a similar procedure as that for **L1** using 9-anthraldehyde (0.9 g, 4.65 mmol), 4-(2,2':6',2''-terpyridyl-4')-benzyl triphenylphosphonium bromide (1.0 g, 3.10 mmol) and potassium *tert*-butoxide (2.08 g, 18.60 mmol) and 35 ml of dry THF. The pure product was isolated as bright yellow solid. Yield: 0.32 g (51%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.04 (d, *J* = 16.8 Hz, 1H), 7.37-7.40 (m, 2H), 7.47-7.51 (m, 4H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.89-7.93 (m, 4H), 8.02-8.06 (m, 4H), 8.39-8.43 (m, 3H), 8.68-8.77 (m, 4H, Py), 8.83 (s, 2H, Py); $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 118.9, 121.6, 124.0, 124.3, 125.5,126.4, 126.9, 127.4, 127.7, 127.9, 128.4, 128.9, 129.3, 129.9, 131.8, 132.7, 137.1, 138.1, 149.4, 149.9, 156.2, 156.5; LCMS (ESI^+): $C_{37}H_{28}N_3$, Calculated value 512.2 ($[M+H]^+$); experimental 512.4 ($[M+H]^+$); FTIR (KBr, cm^{-1}): 2924 ($\bar{\upsilon}_{\text{C-H stretching}}$), 1584 ($\bar{\upsilon}_{\text{C=C stretching}}$), 1569 ($\bar{\upsilon}_{\text{C=N stretching}}$); $\lambda_{max}(\varepsilon)$: 391 nm ($\varepsilon = 1.5\times10^4$ $M^{-1}cm^{-1}$), 286 nm ($\varepsilon = 3.1\times10^4$ $M^{-1}cm^{-1}$); λ_{em}: 498 nm (λ_{ex}: 391 nm).

1b. NMR Spectra

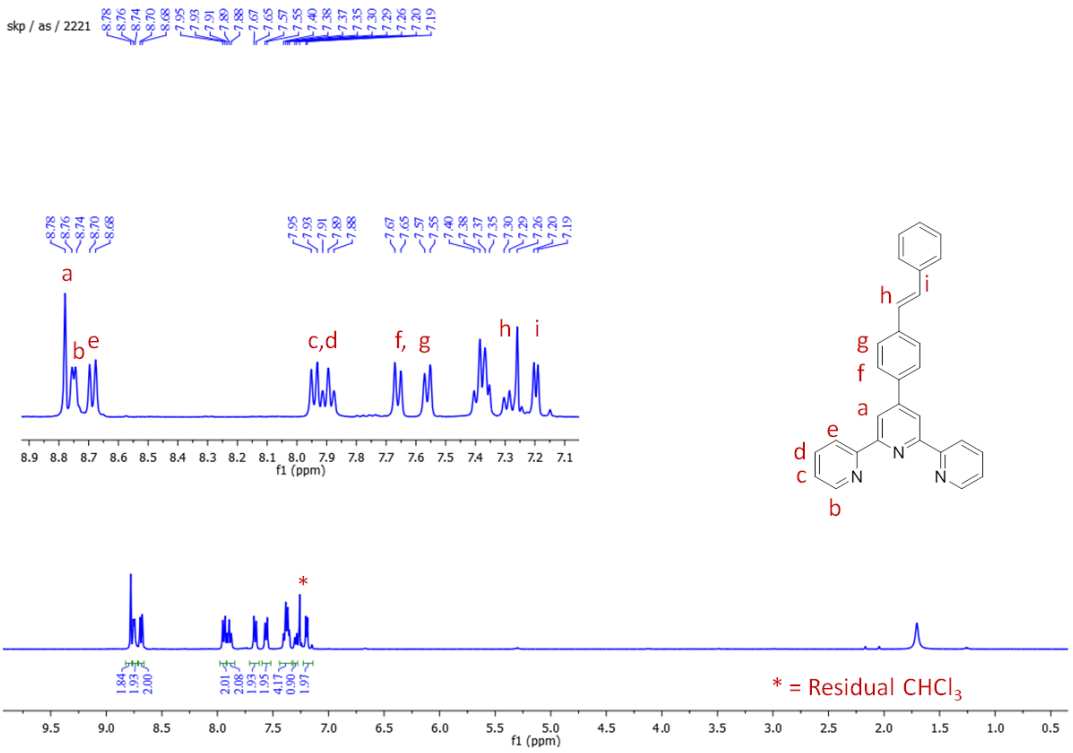

Fig. S1: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **L1**; proton marked as h and one of the vinyl protons (i) are overlapped.

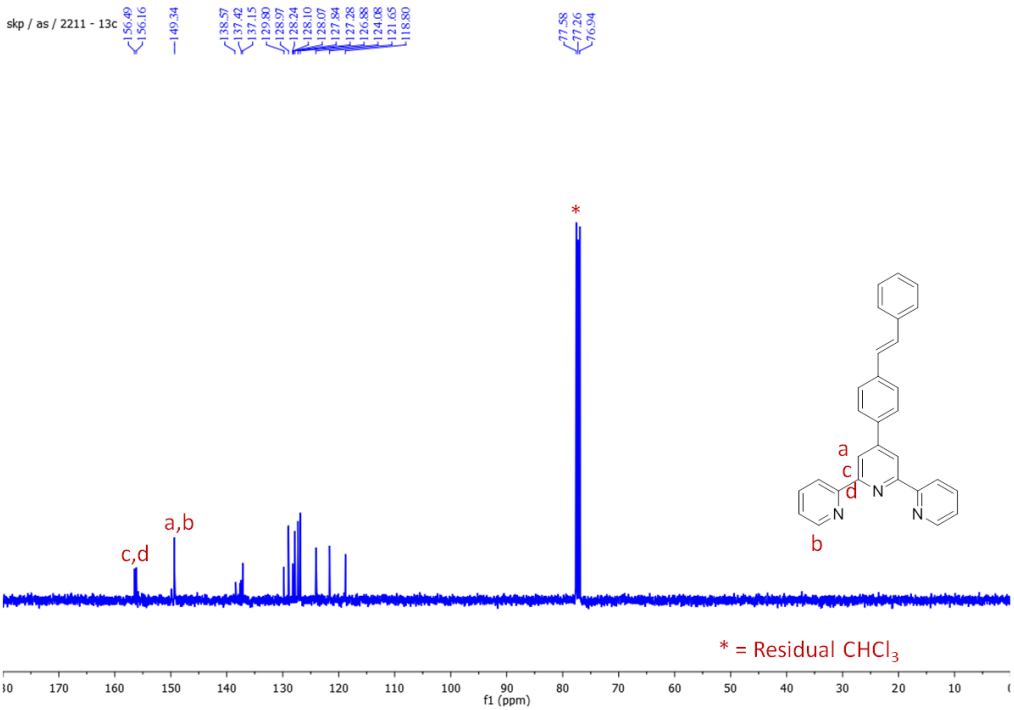

Fig. S2: $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **L1**

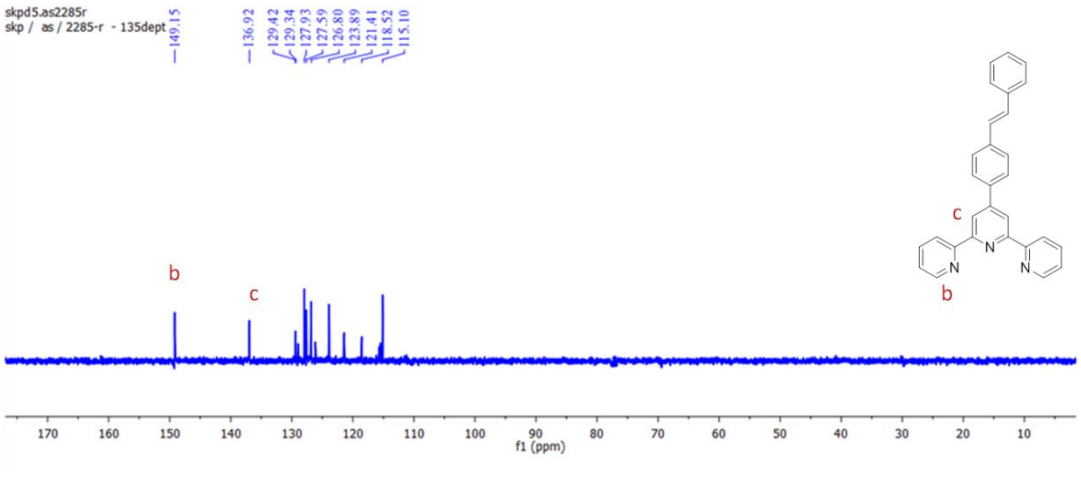

Fig. S3: DEPT-135 NMR (100 MHz, $CDCl_3$) spectrum of **L1**

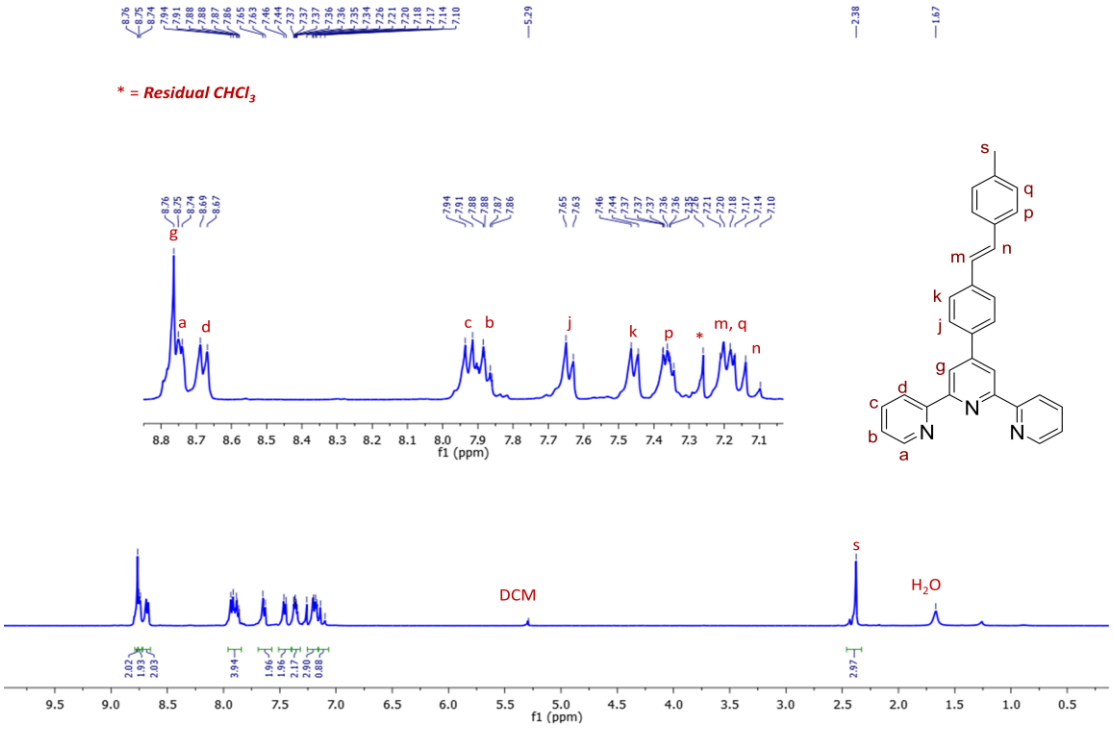

Fig. S4: ^1H NMR (400 MHz, $CDCl_3$) spectrum of **L2**; proton marked as q and one of the vinyl protons (m) are overlapped.

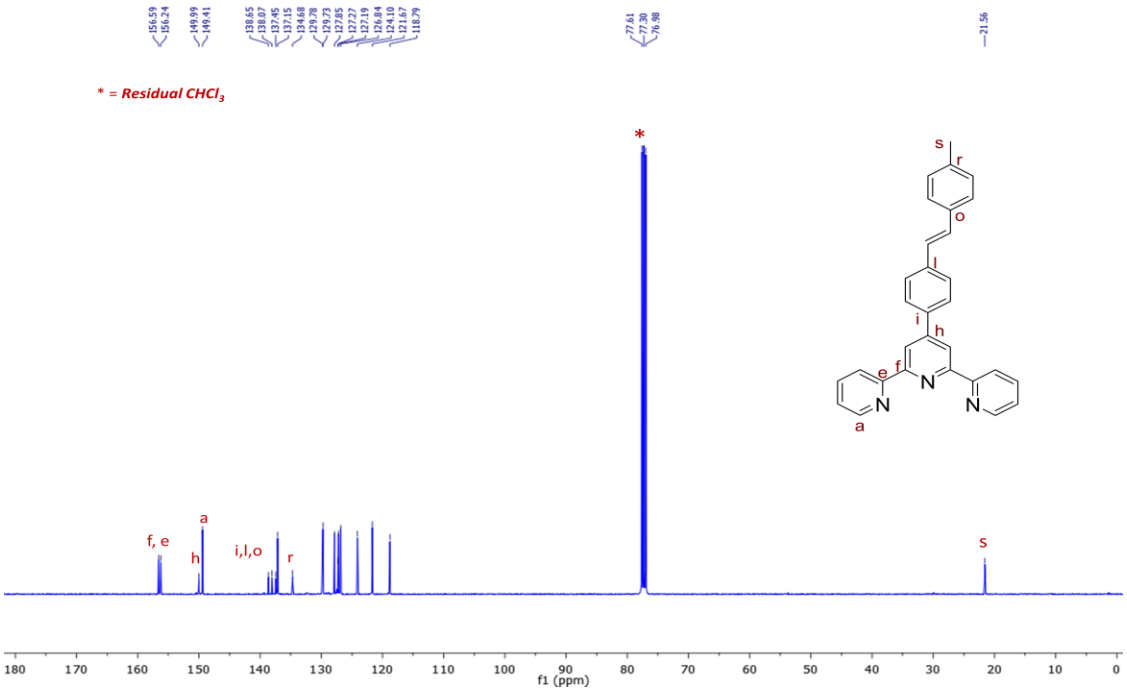

Fig. S5: $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **L2**

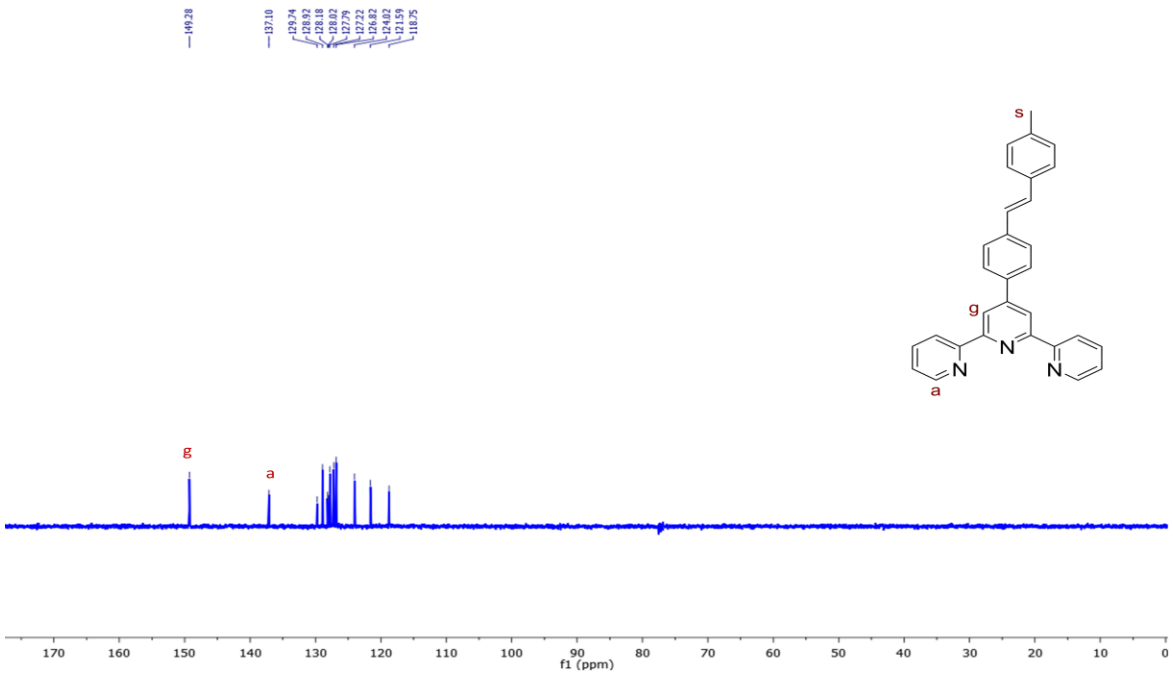

Fig. S6: DEPT-135 NMR (100 MHz, $CDCl_3$) spectrum of **L2**

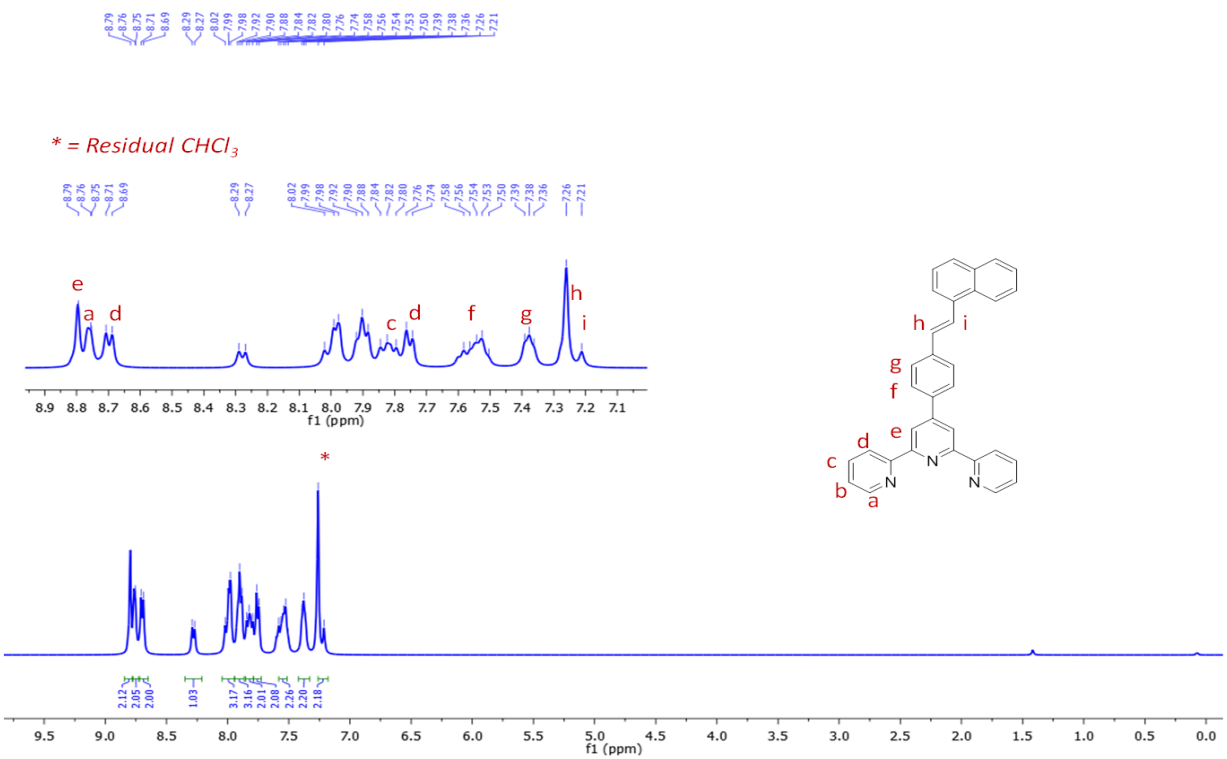

Fig. S7: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **L3**; proton marked as 'h' is one of the vinyl protons, which is overlapped with residual $CHCl_3$.

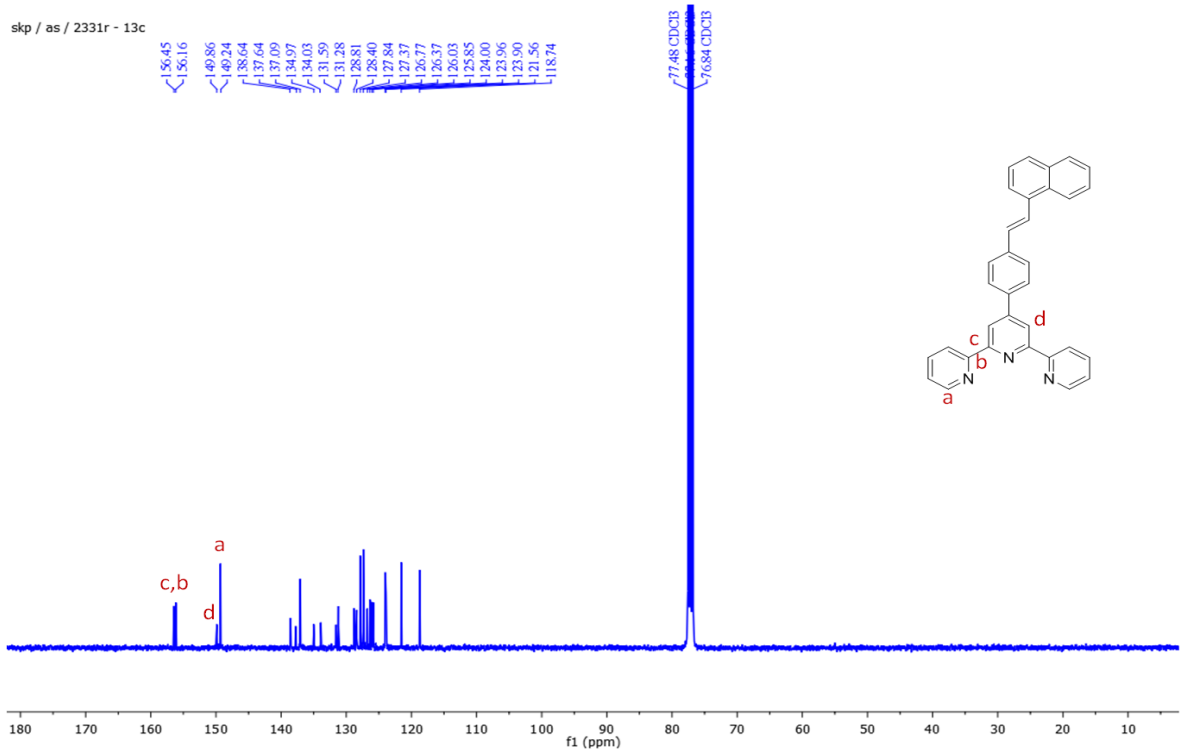

Fig. S8: $^{13}C\{^{1}H\}$NMR (100 MHz, $CDCl_3$) spectrum of **L3**

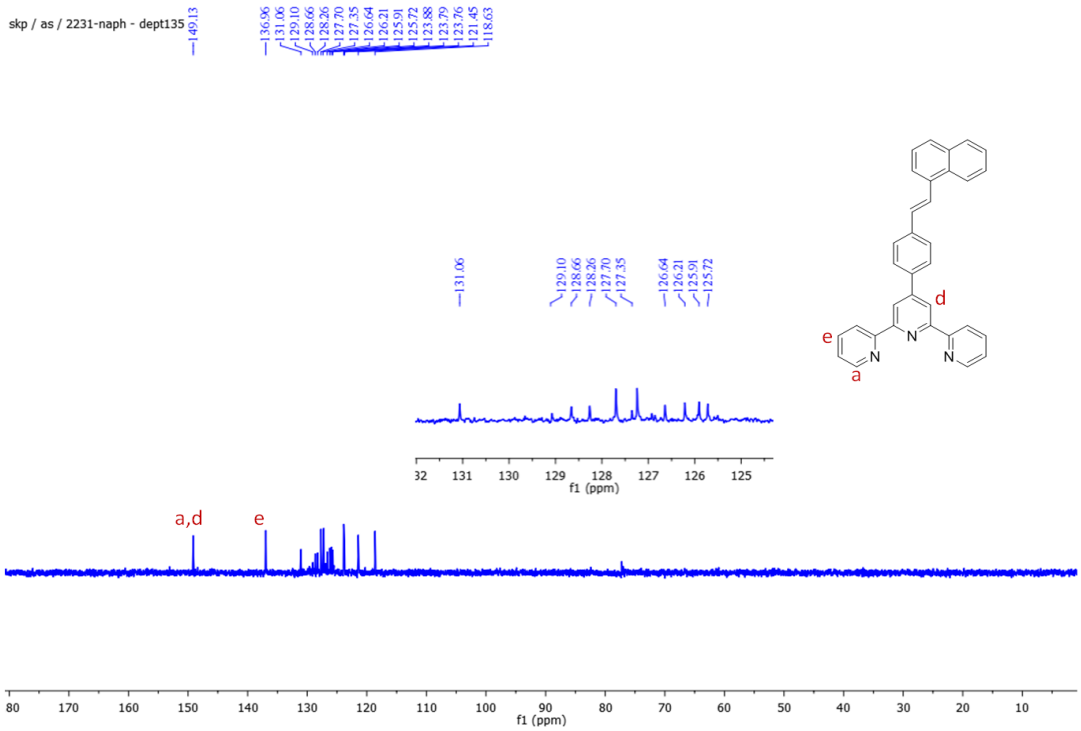

Fig. S9: DEPT-135 NMR (100 MHz, $CDCl_3$) spectrum of **L3**

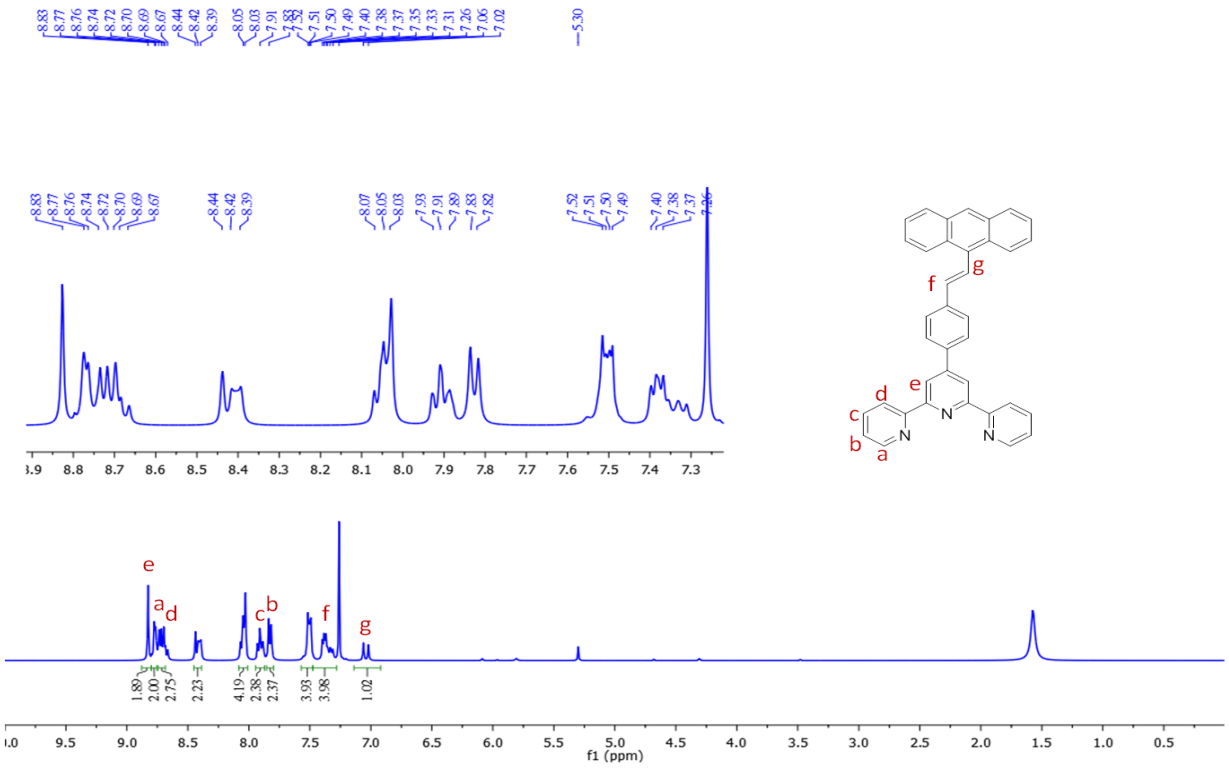

Fig. S10: ^1H NMR (400 MHz, $CDCl_3$) spectrum of **L4**; proton marked as f is one of the vinyl proton which is overlapped with other aromatic protons.

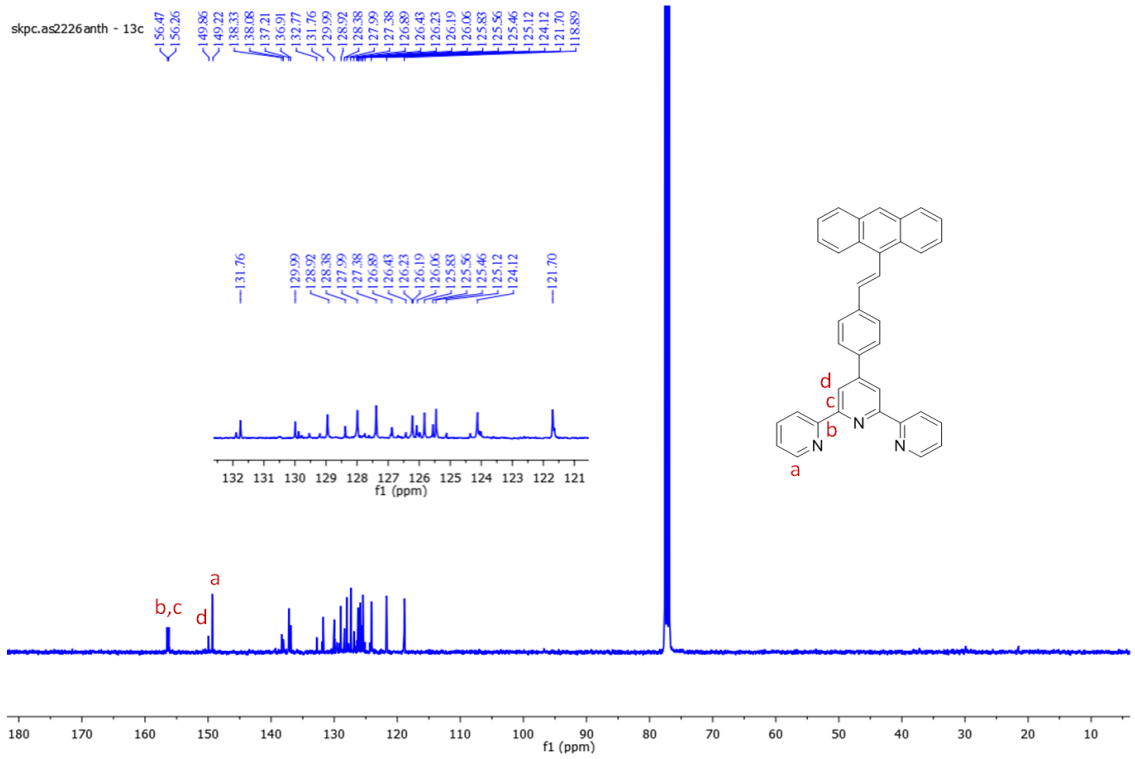

Fig. S11: $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **L4**

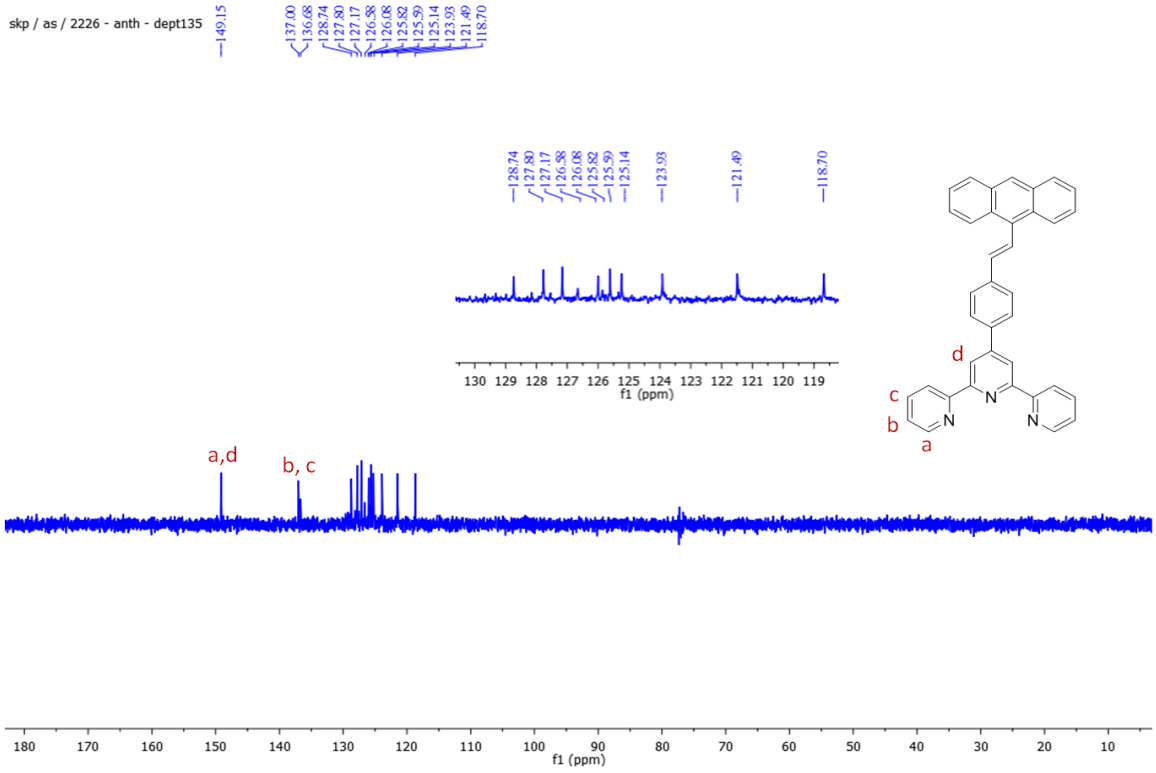

Fig. S12: DEPT-135 NMR (100 MHz, $CDCl_3$) spectrum of **L4**

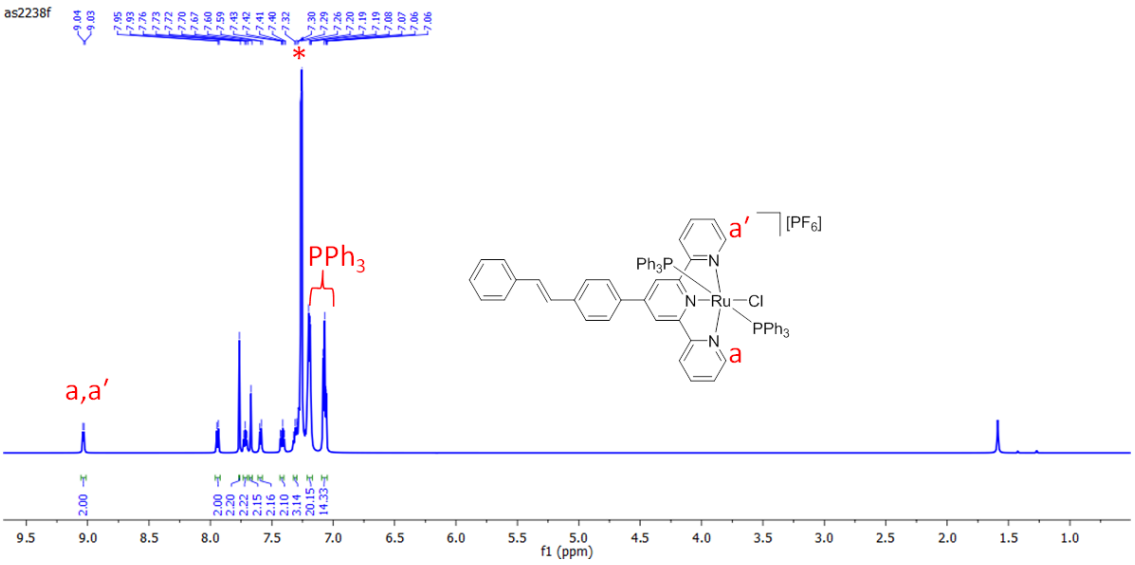

Fig. S13: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **1**

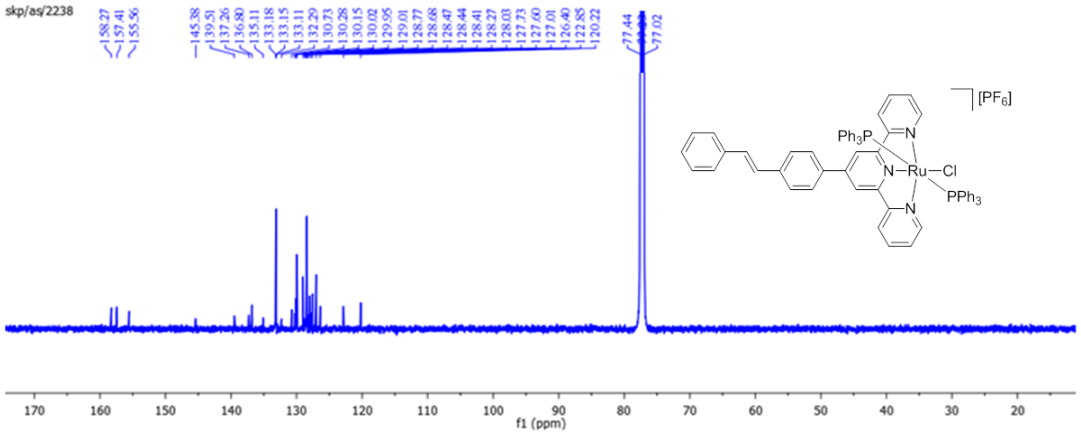

Fig. S14: ^{13}C{^{1}H }NMR (150 MHz, $CDCl_3$) spectrum of **1**

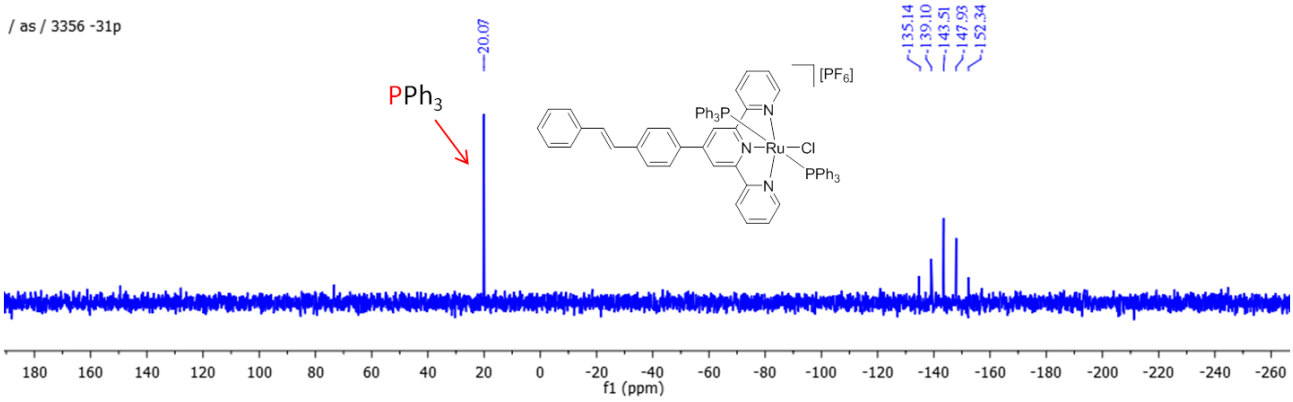

Fig. S15: ^{31}P{^{1}H }NMR (162 MHz, $CDCl_3$) spectrum of **1**

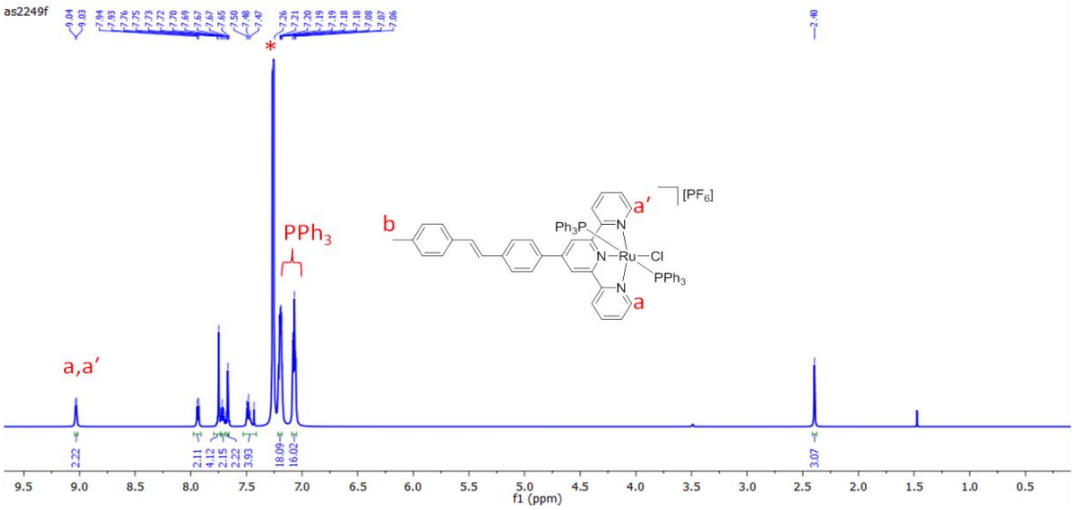

Fig. S16: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **2**

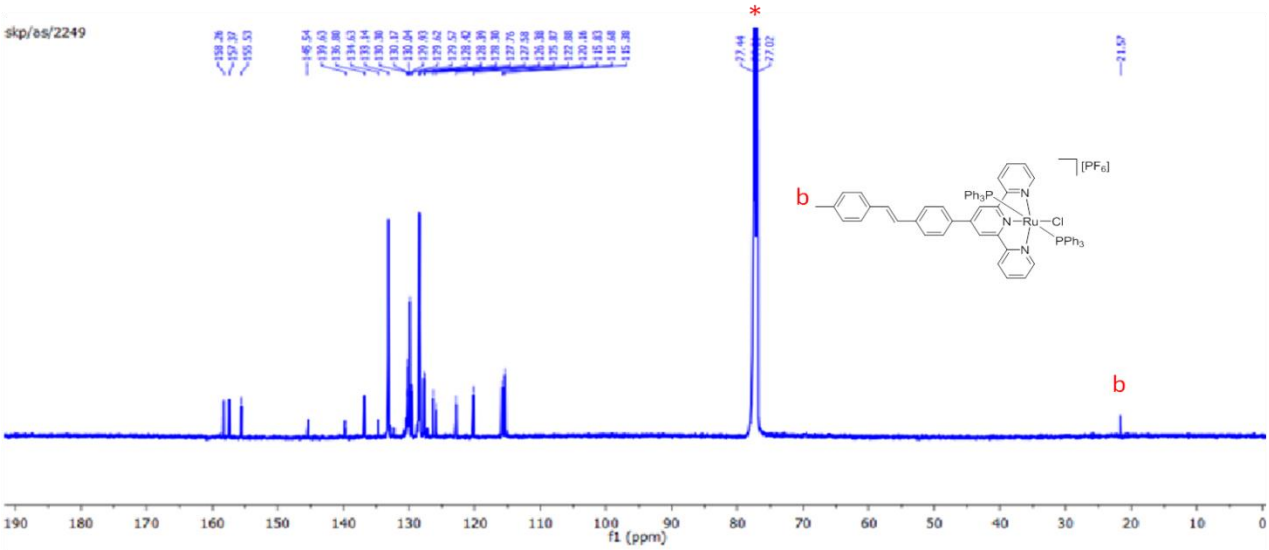

Fig. S17: ^{13}C{^{1}H }NMR (150 MHz, $CDCl_3$) spectrum of **2**

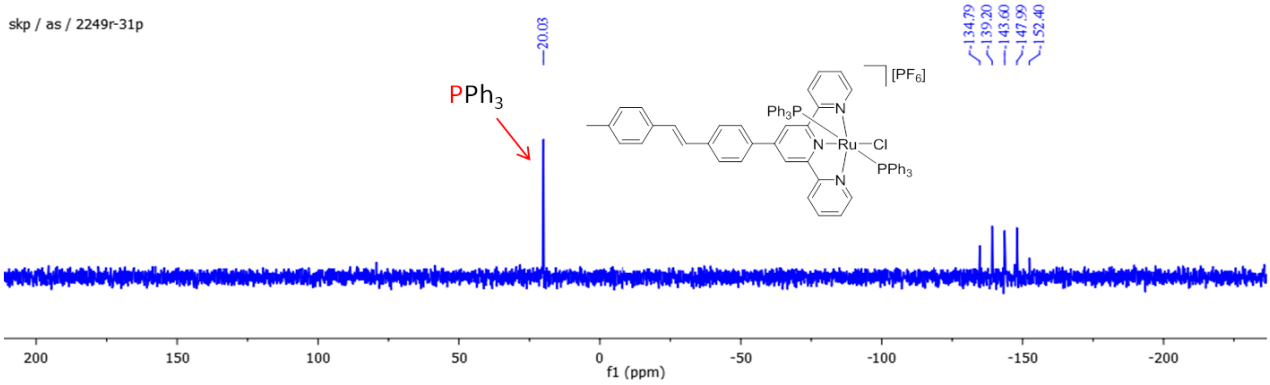

Fig. S18: ^{31}P{^{1}H }NMR (162 MHz, $CDCl_3$) spectrum of **2**

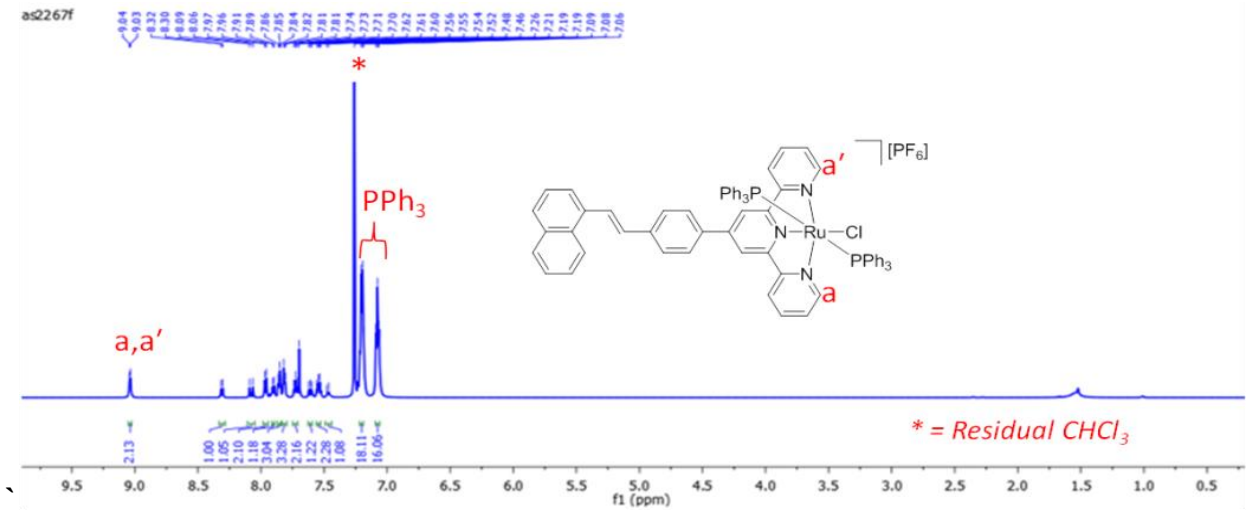

Fig. S19: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3**

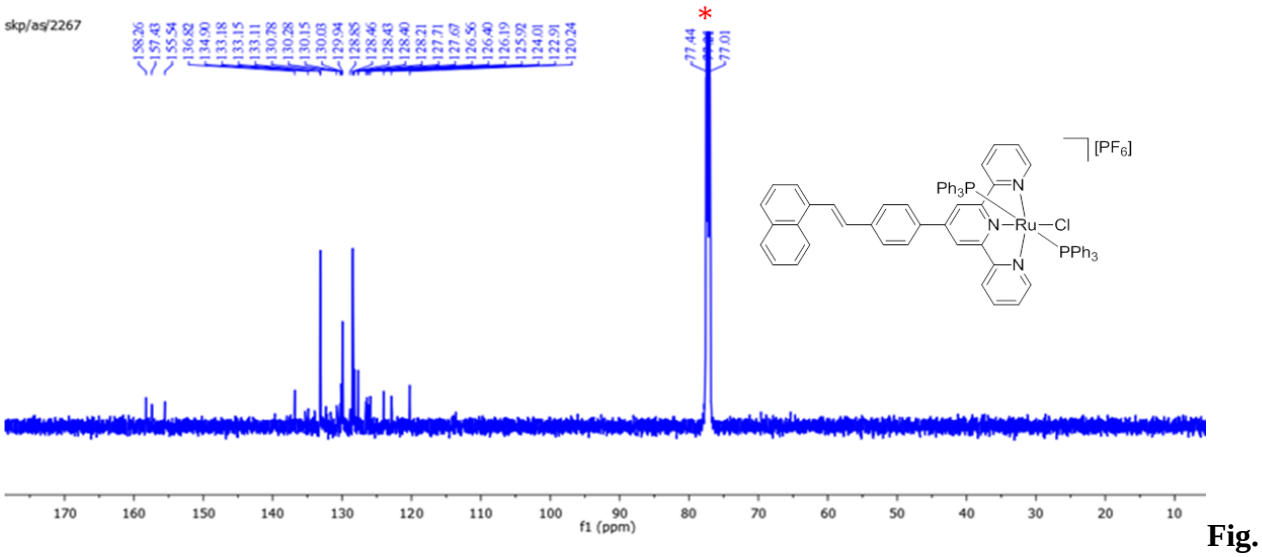

Fig. S20: ^{13}C{^{1}H }NMR (150 MHz, $CDCl_3$) spectrum of **3**

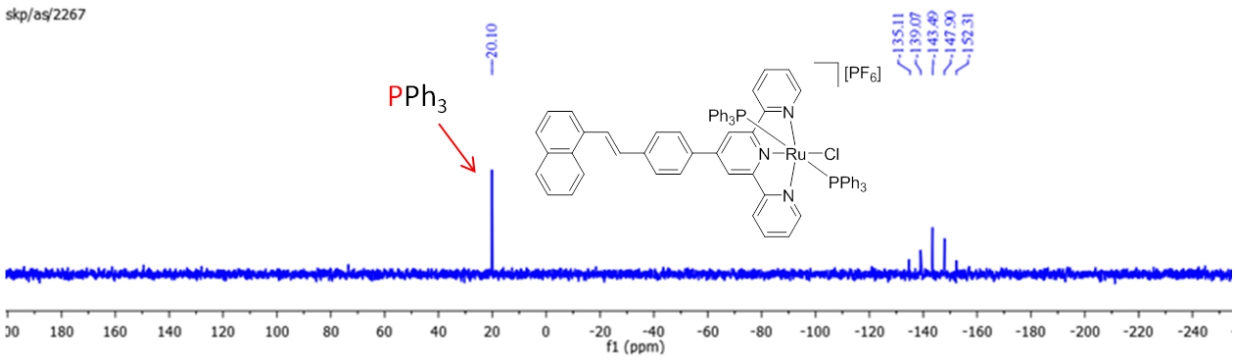

Fig. S21: ^{31}P{^{1}H }NMR (162 MHz, $CDCl_3$) spectrum of **3**

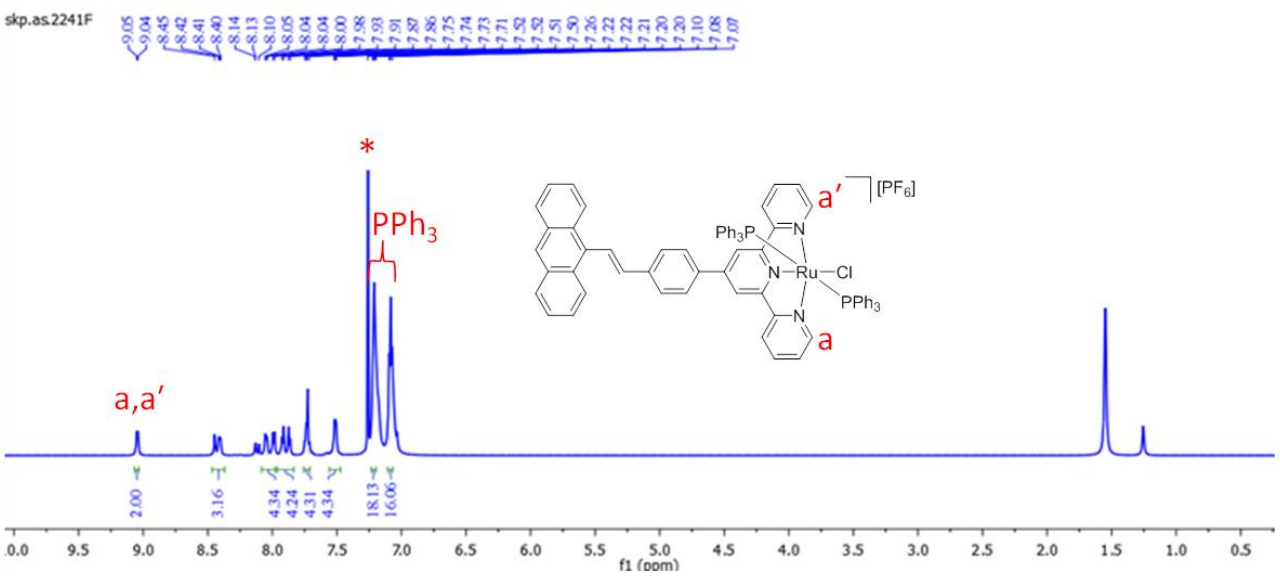

Fig. S22: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3**

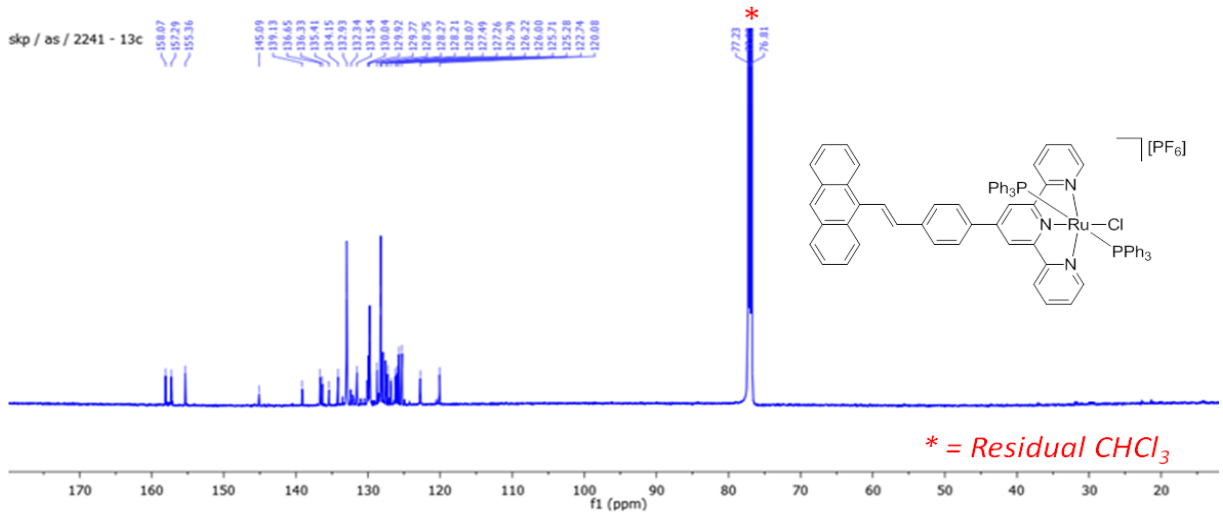

Fig. S23: ^{13}C{^{1}H }NMR (150 MHz, $CDCl_3$) spectrum of **4**

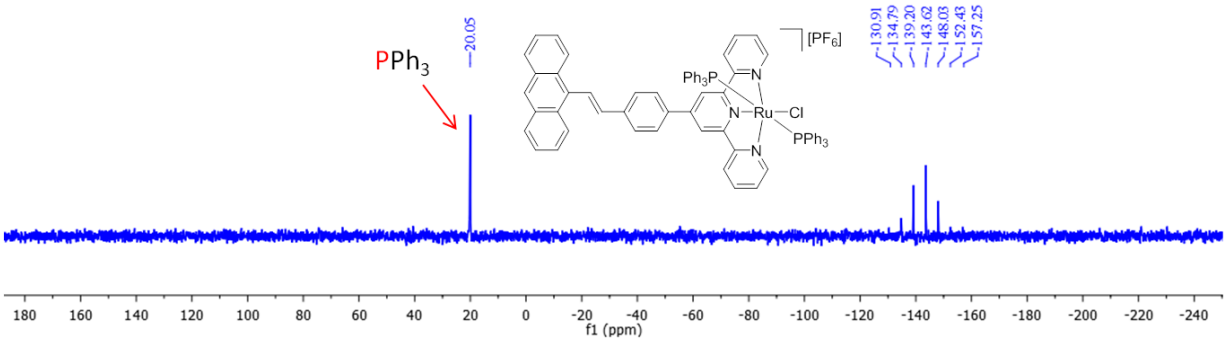

Fig. S24: ^{31}P{^{1}H }NMR (162 MHz, $CDCl_3$) spectrum of **4**

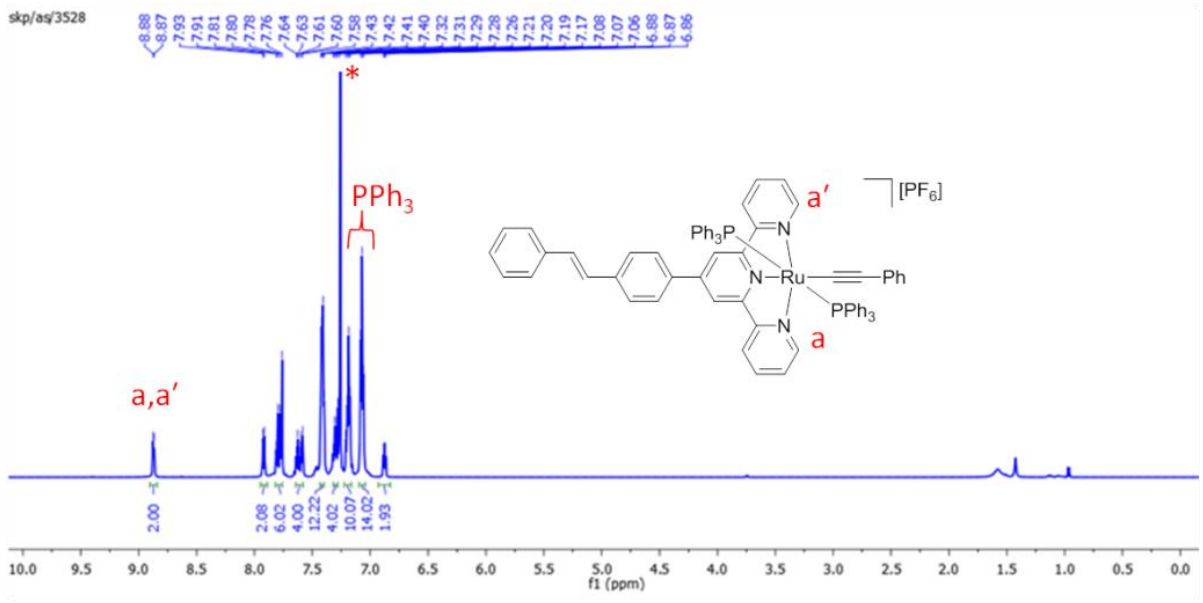

Fig. S25: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **5**

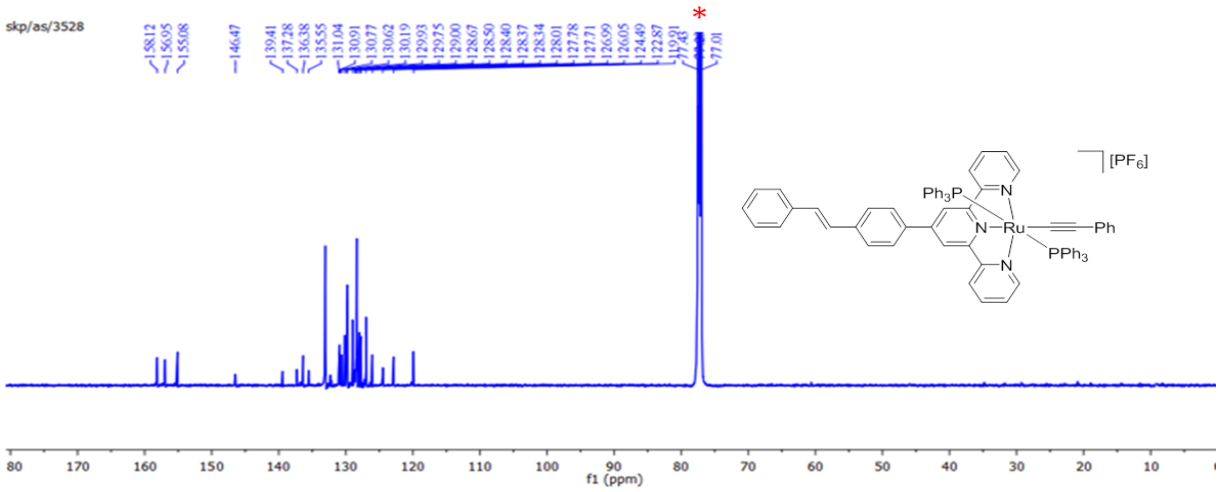

Fig. S26: ^{13}C{^{1}H }NMR (150 MHz, $CDCl_3$) spectrum of **5**

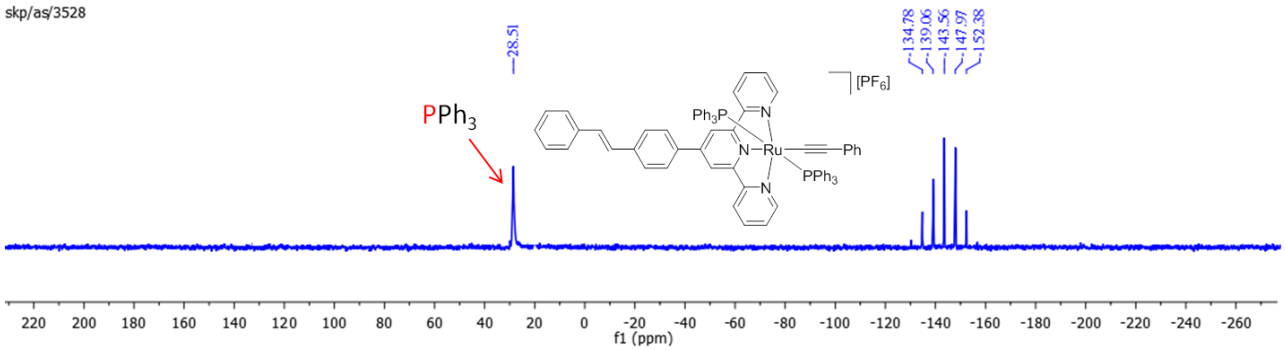

Fig. S27: ^{31}P{^{1}H }NMR (162 MHz, $CDCl_3$) spectrum of **5**

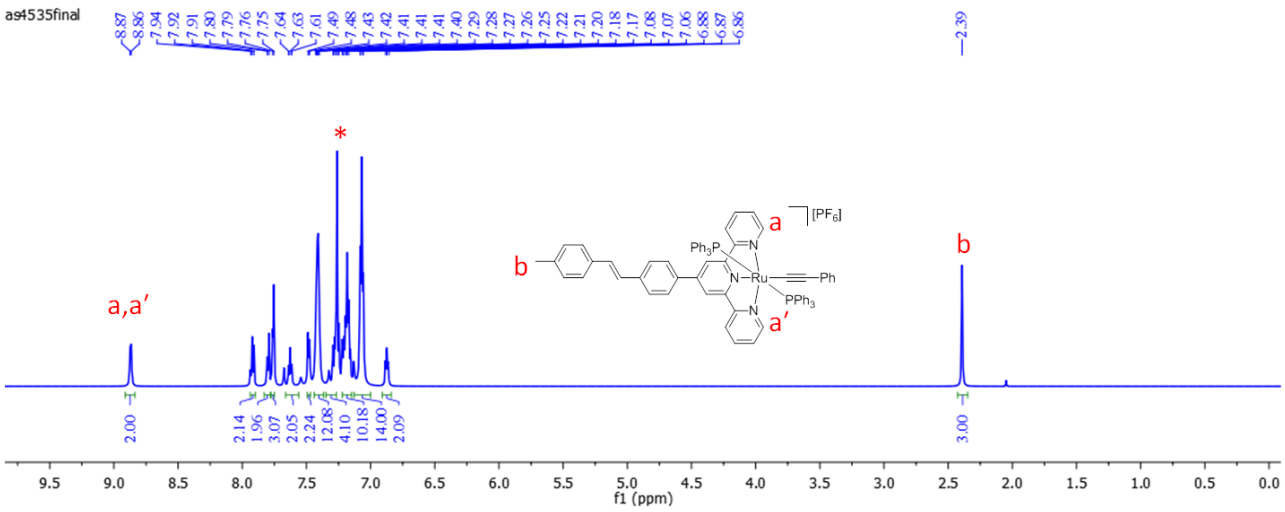

Fig. S28: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **5**

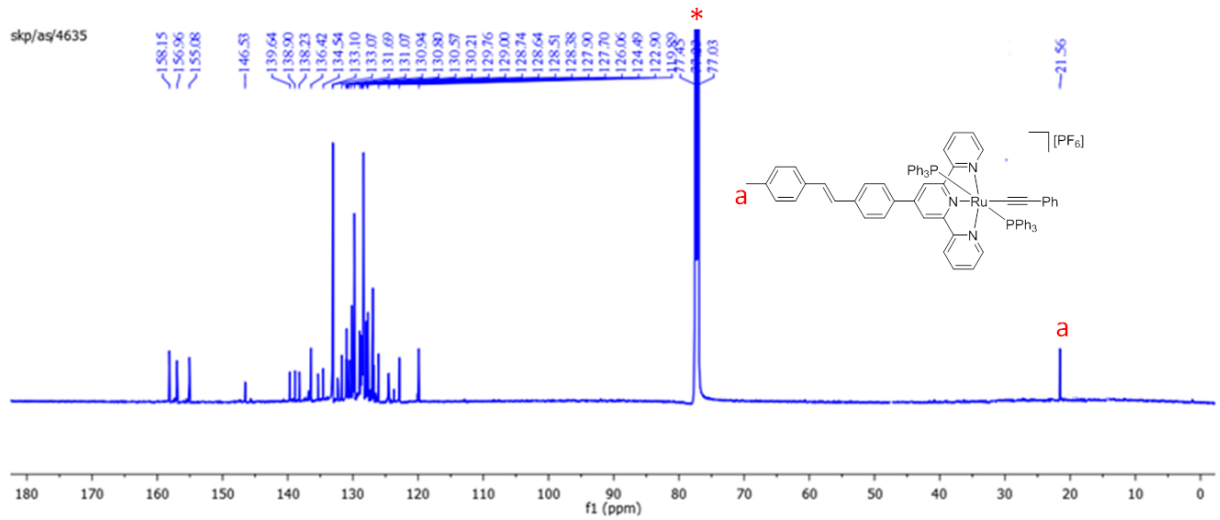

Fig. S29: $^{13}C\{^{1}H\}$NMR (150 MHz, $CDCl_3$) spectrum of **6**

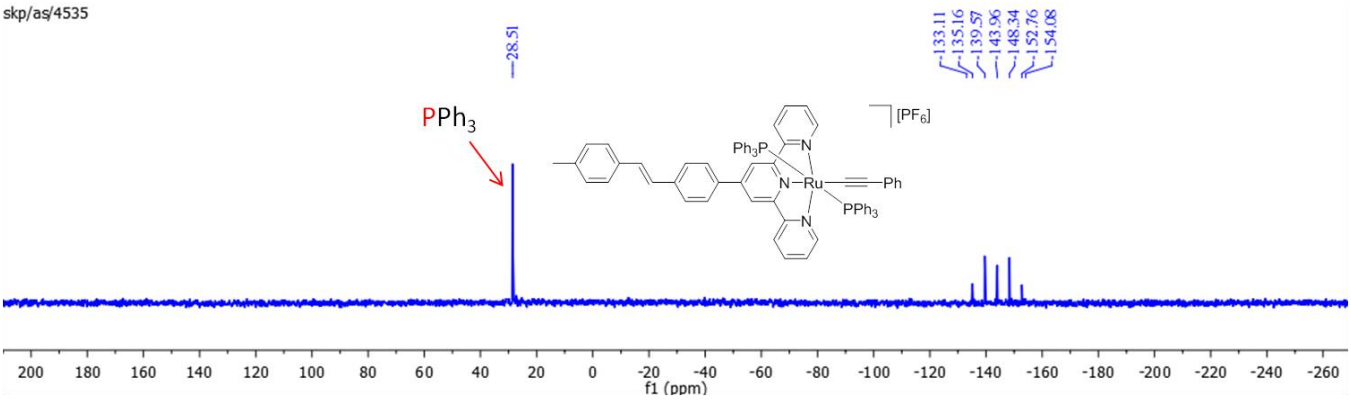

Fig. S30: $^{31}P\{^{1}H\}$NMR (162 MHz, $CDCl_3$) spectrum of **6**

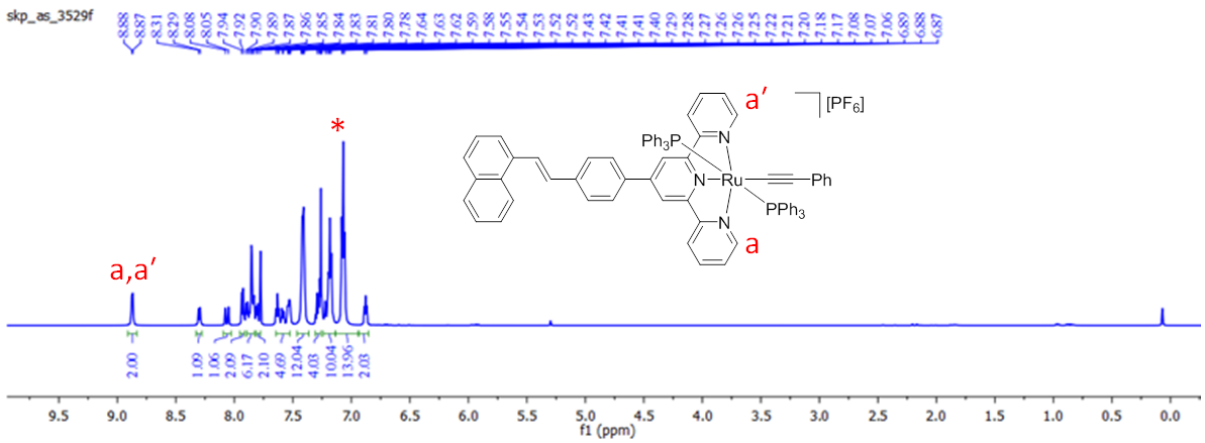

Fig. S31: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **7**

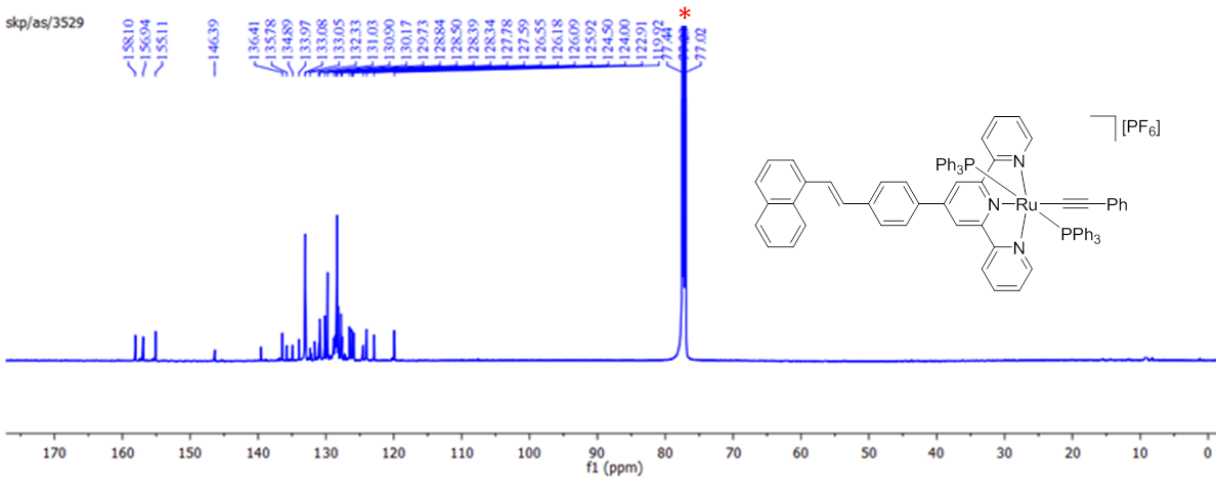

Fig. S32: ^{13}C{^{1}H }NMR (150 MHz, $CDCl_3$) spectrum of **7**

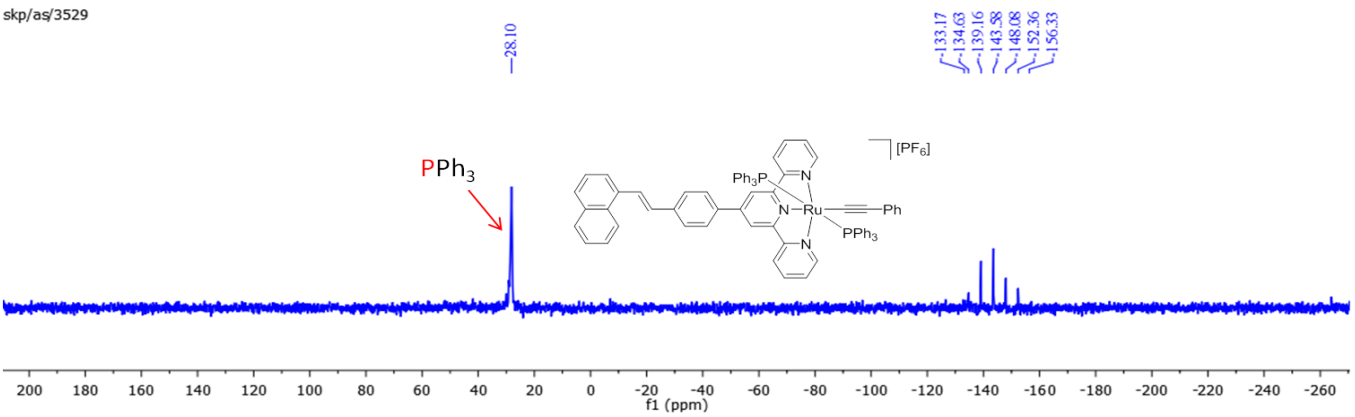

Fig. S33: ^{31}P{^{1}H }NMR (162 MHz, $CDCl_3$) spectrum of **7**

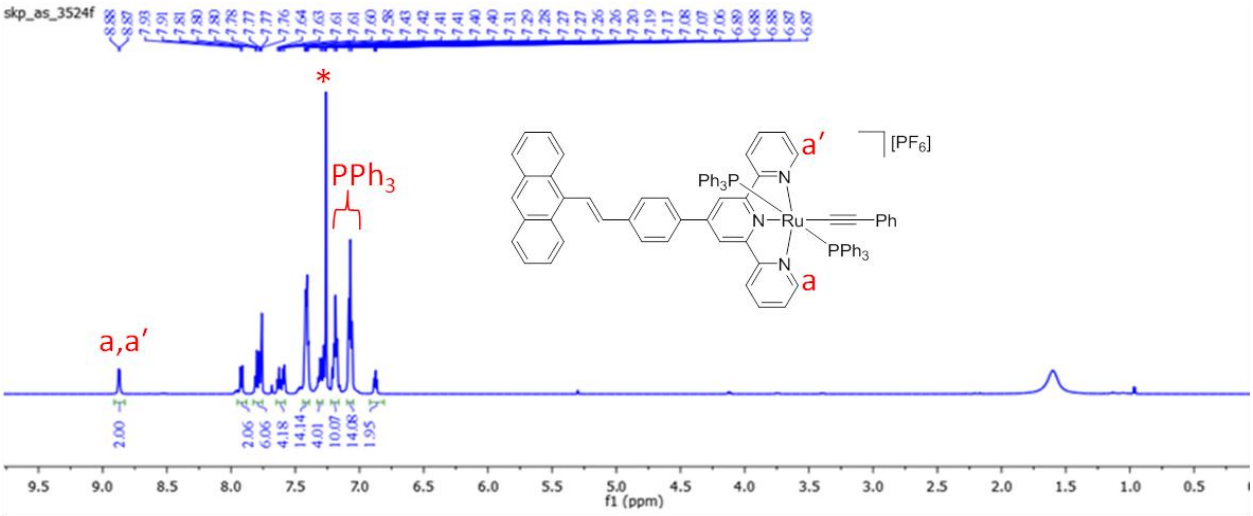

Fig. S34: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **8**

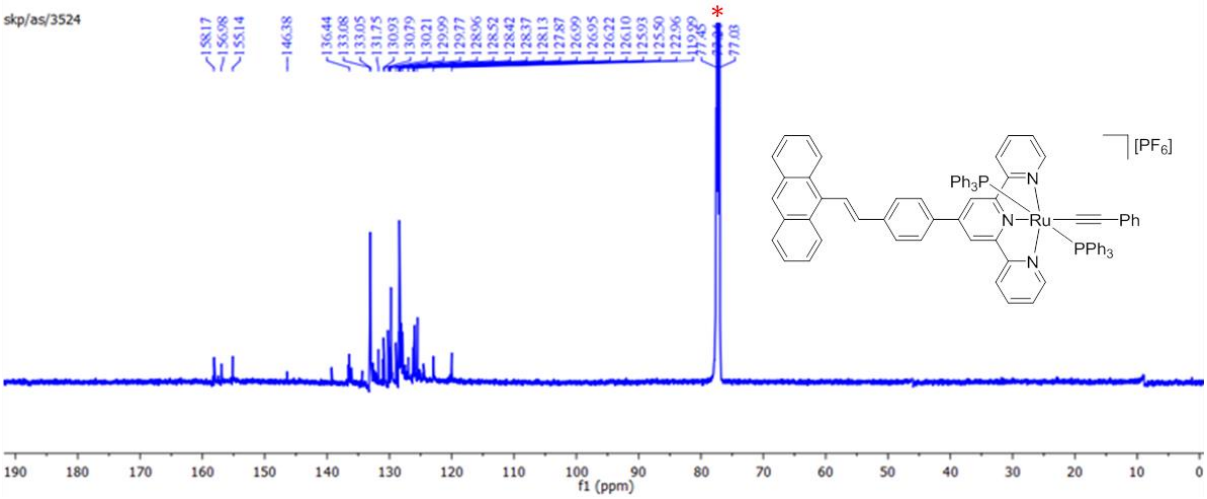

Fig. S35: ^{13}C{^{1}H }NMR (150 MHz, $CDCl_3$) spectrum of **8**

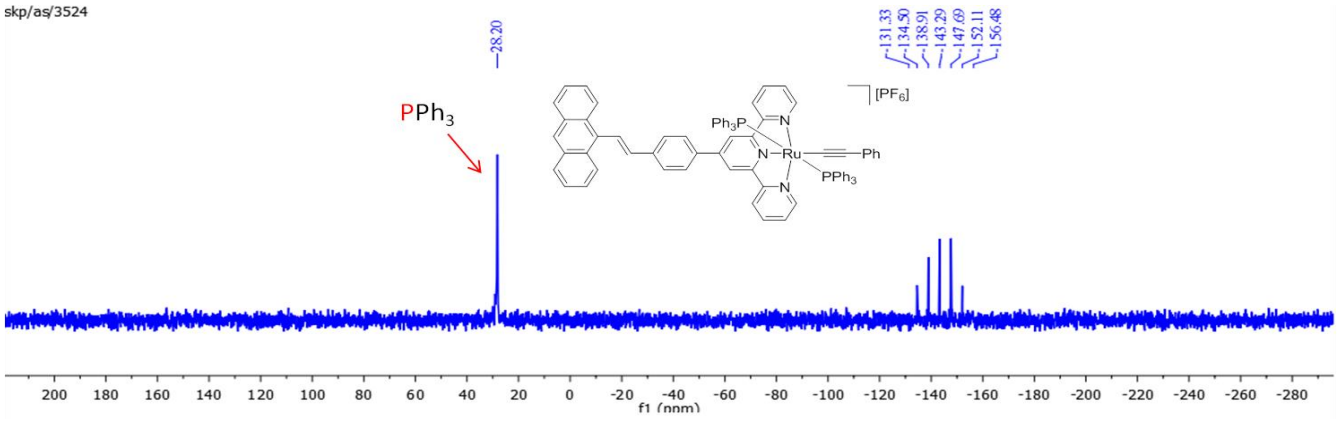

Fig. S36: ^{31}P{^{1}H }NMR (162 MHz, $CDCl_3$) spectrum of **8**

1c. FTIR data (measured as KBr pellets)

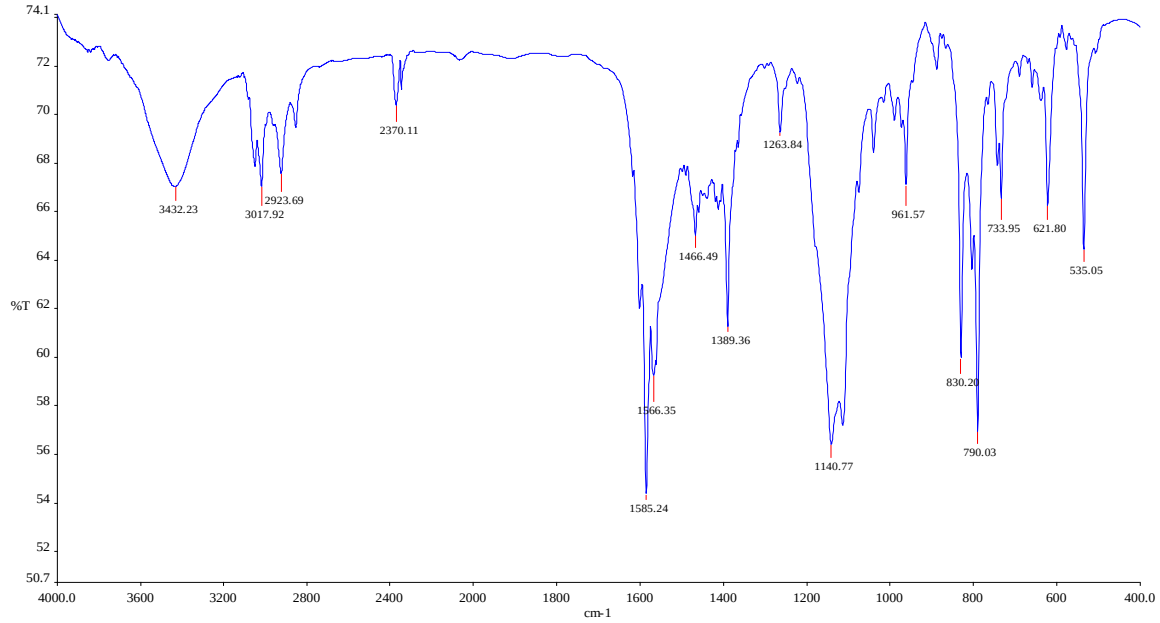

Fig. S37: FTIR spectrum of **L1**

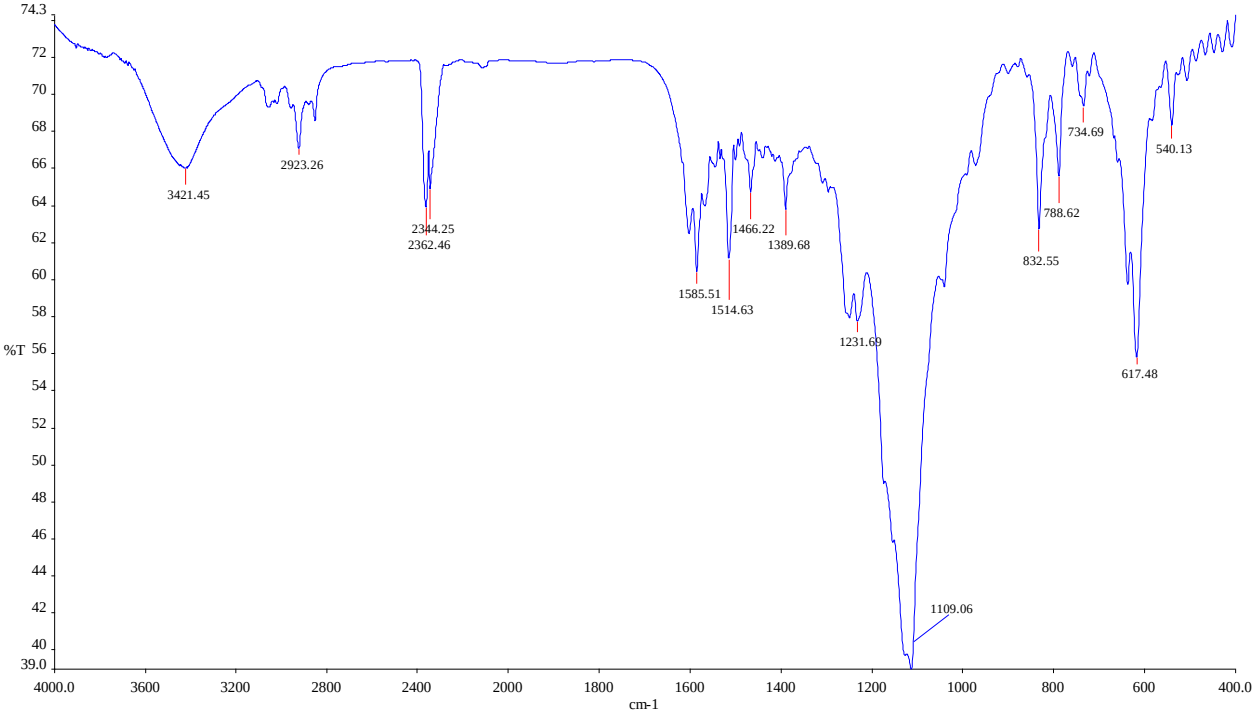

Fig. S38: FTIR spectrum of **L2**

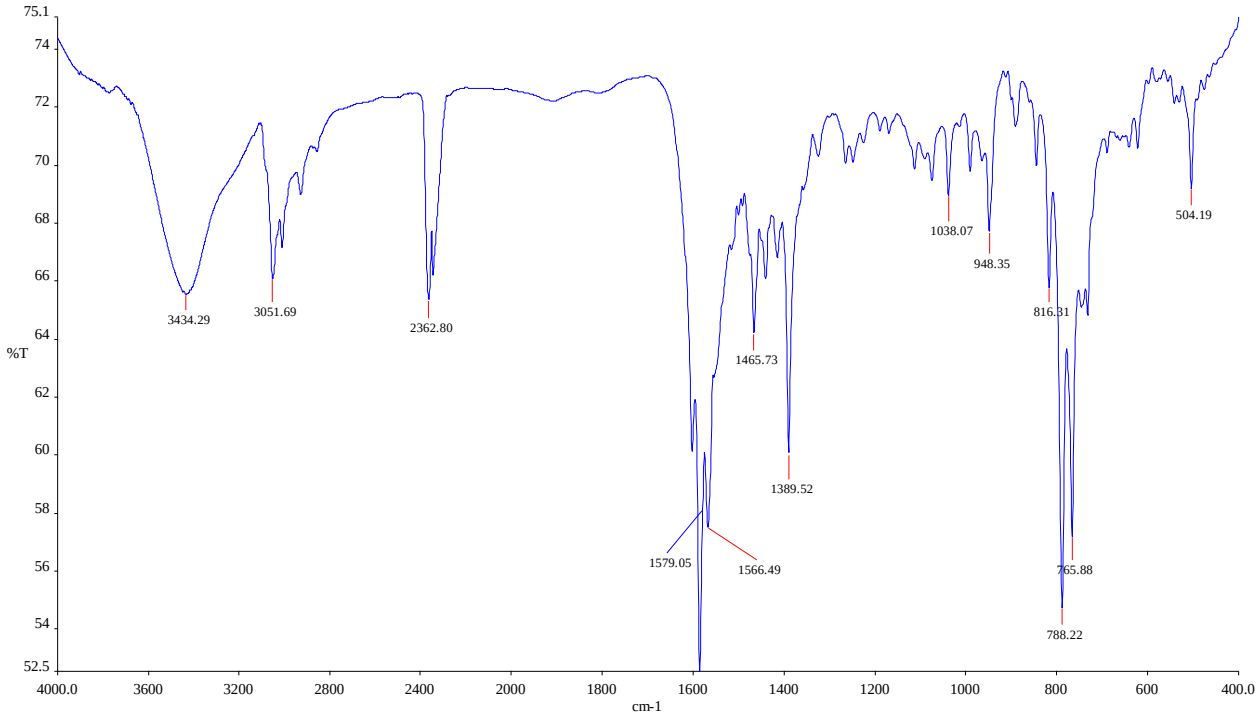

Fig. S39: FTIR spectrum of **L3**

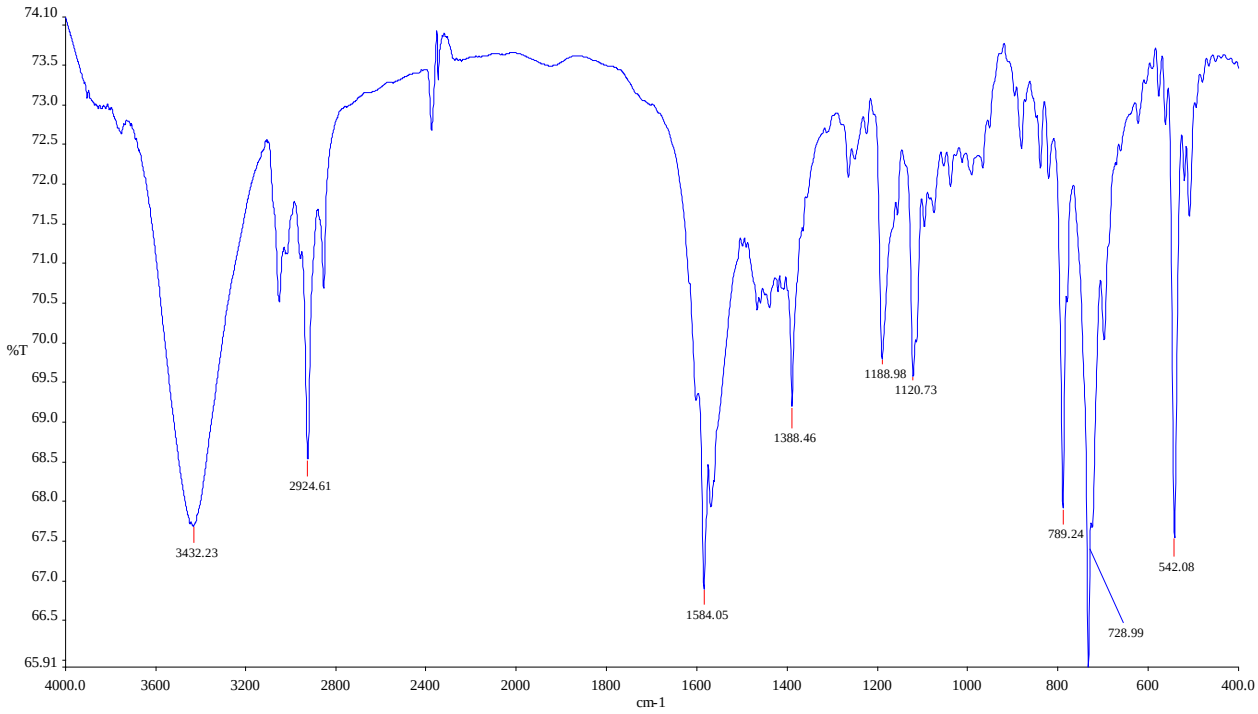

Fig. S40: FTIR spectrum of **L4**

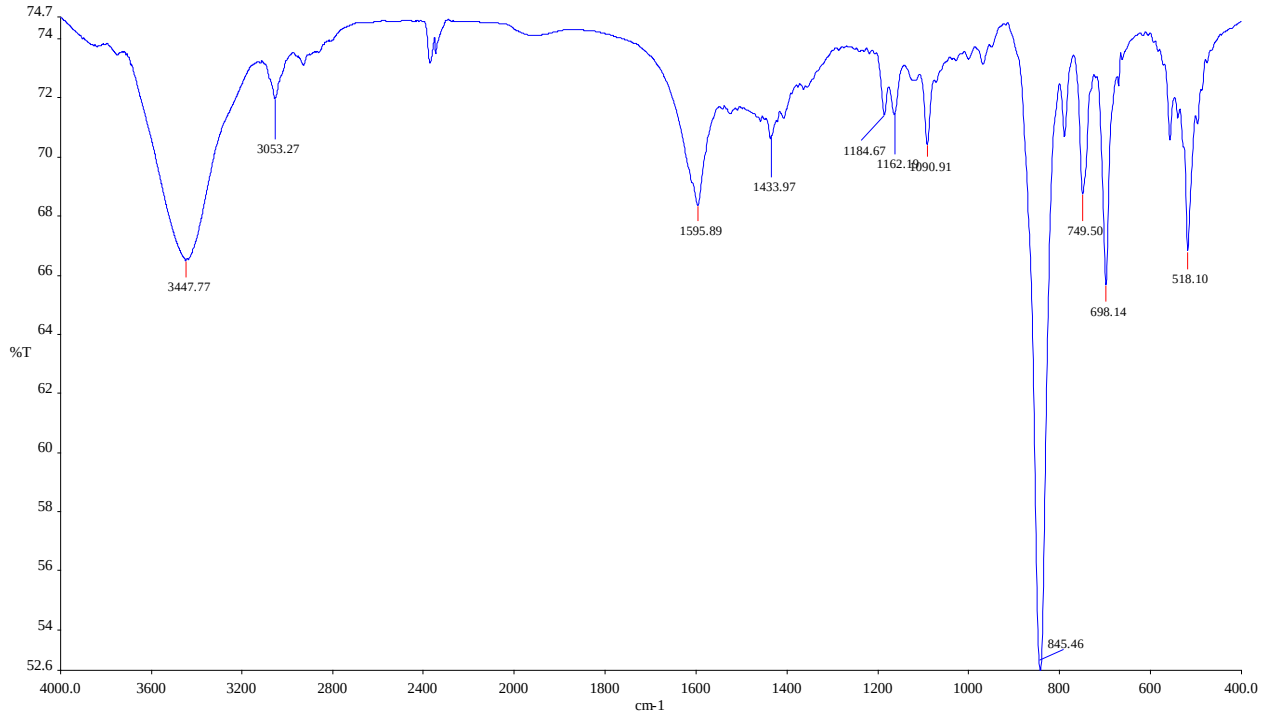

Fig. S41: FTIR spectrum of **1**

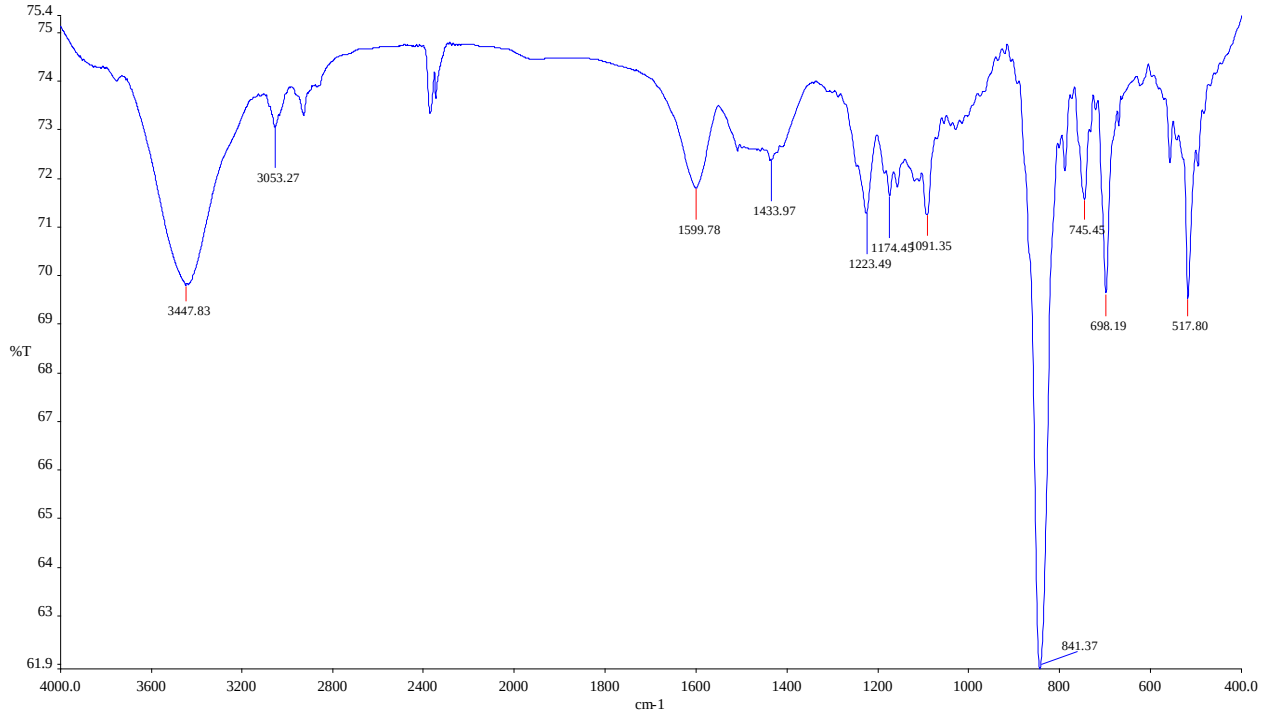

Fig. S42: FTIR spectrum of **2**

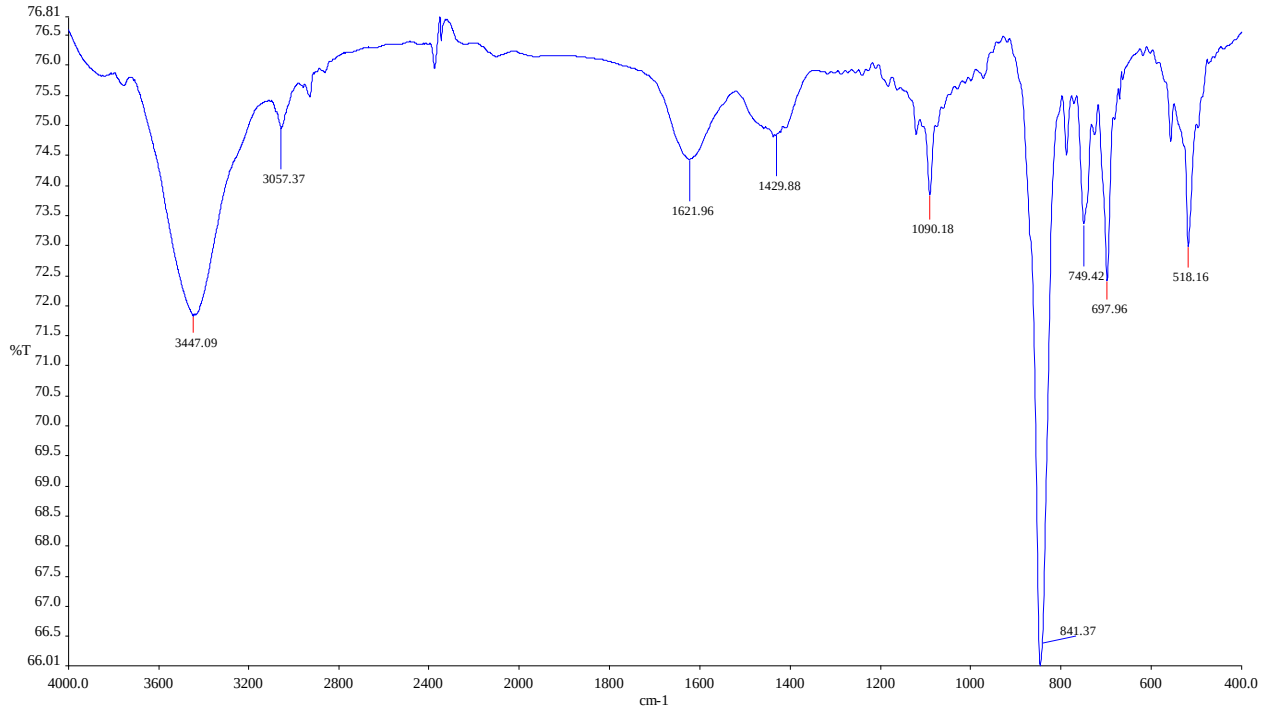

Fig. S43: FTIR spectrum of **3**

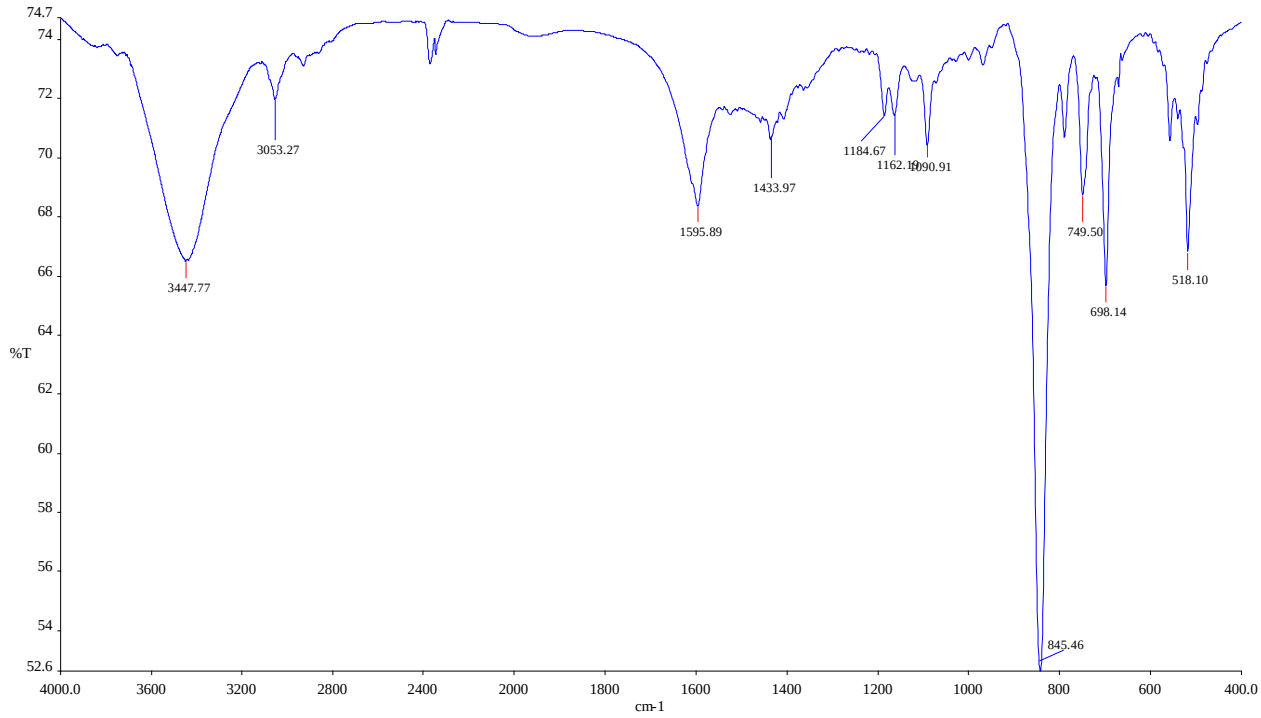

Fig. S44: FTIR spectrum of **4**

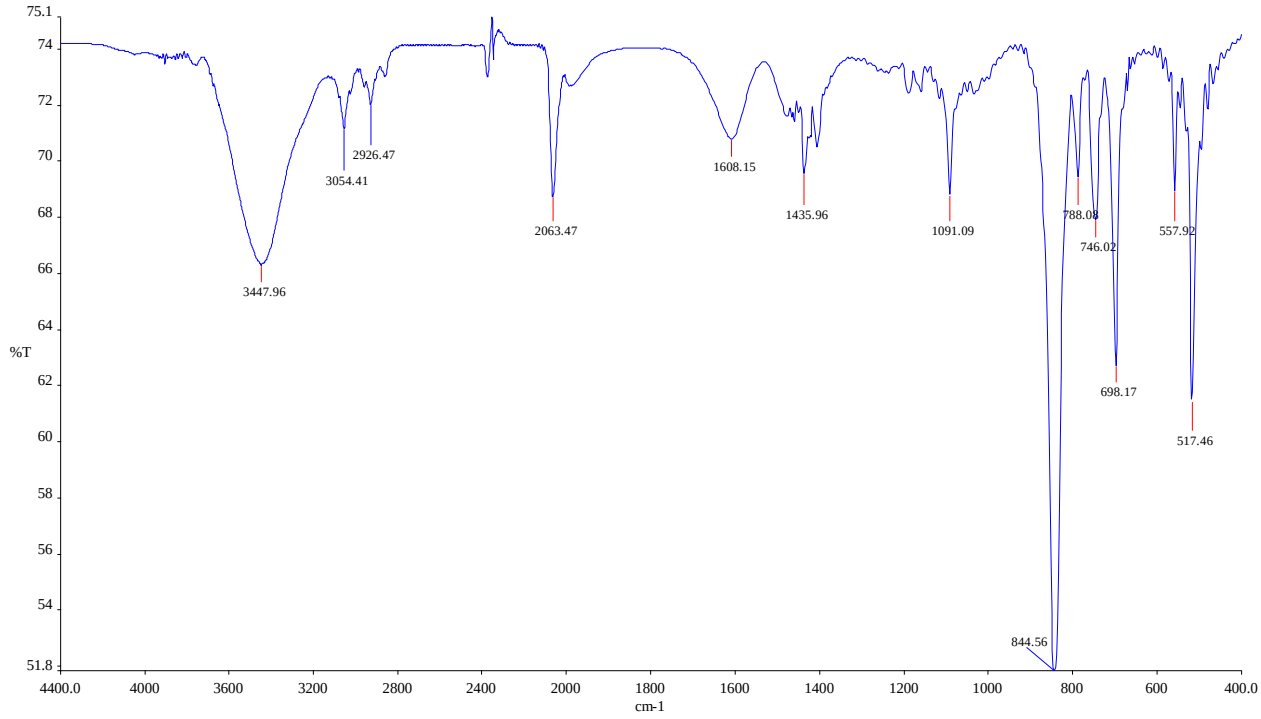

Fig. S45: FTIR spectrum of **5**

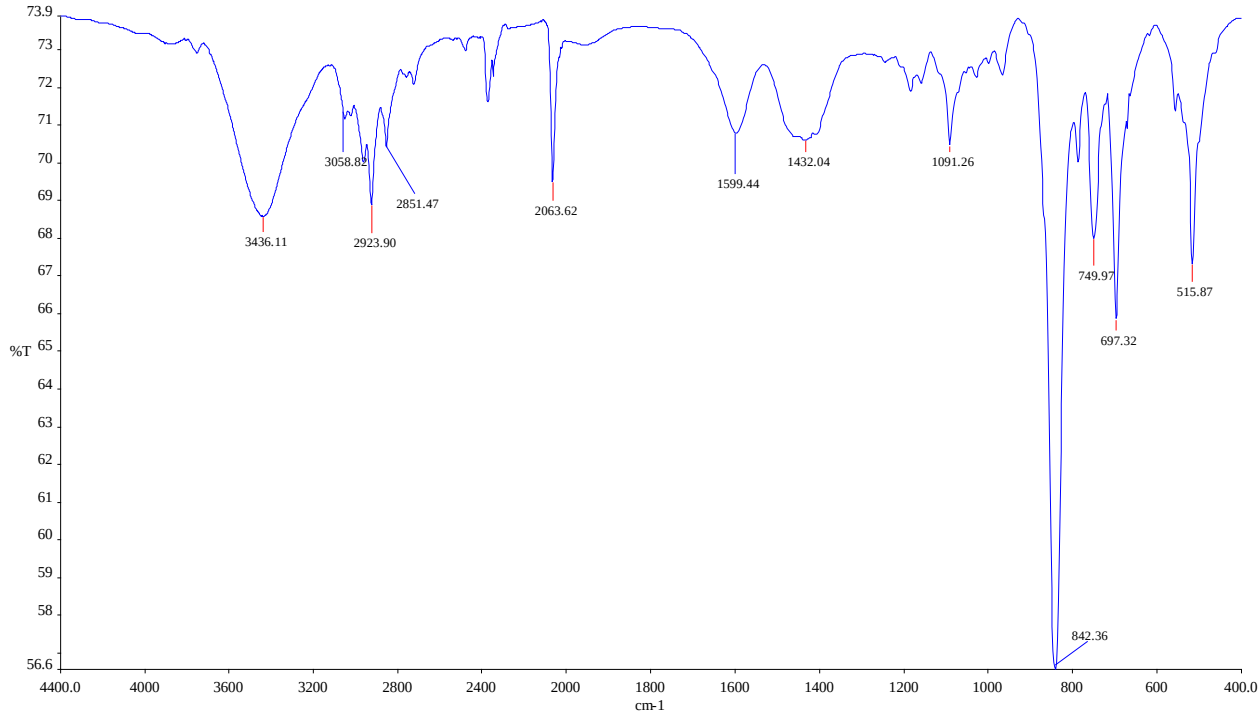

Fig. S46: FTIR spectrum of **6**

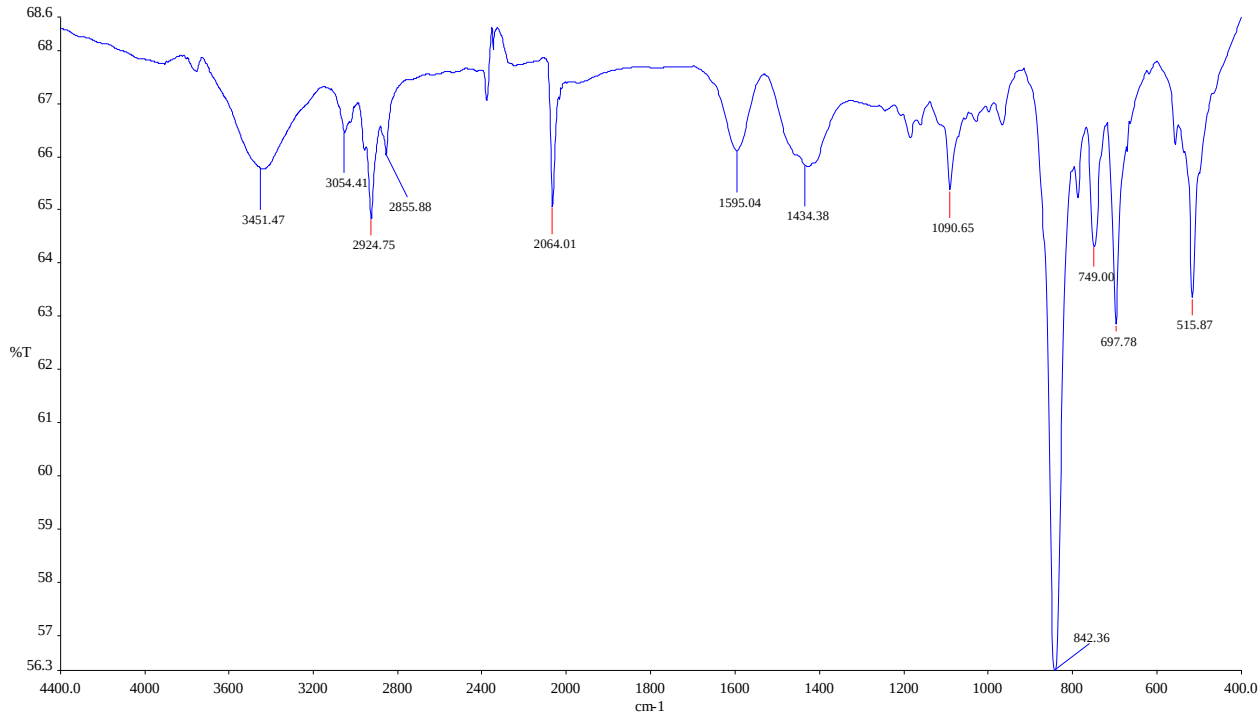

Fig. S47: FTIR spectrum of **7**

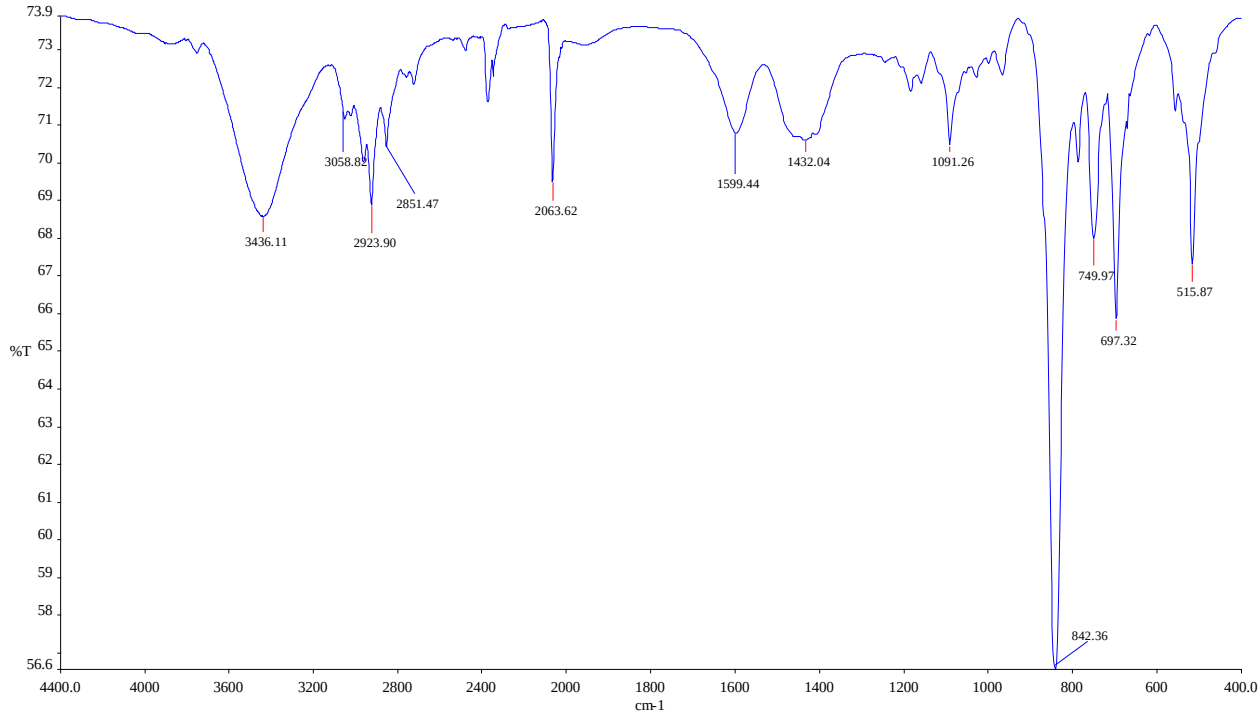

Fig. S48: FTIR spectrum of **8**

1d. Mass spectrometry data

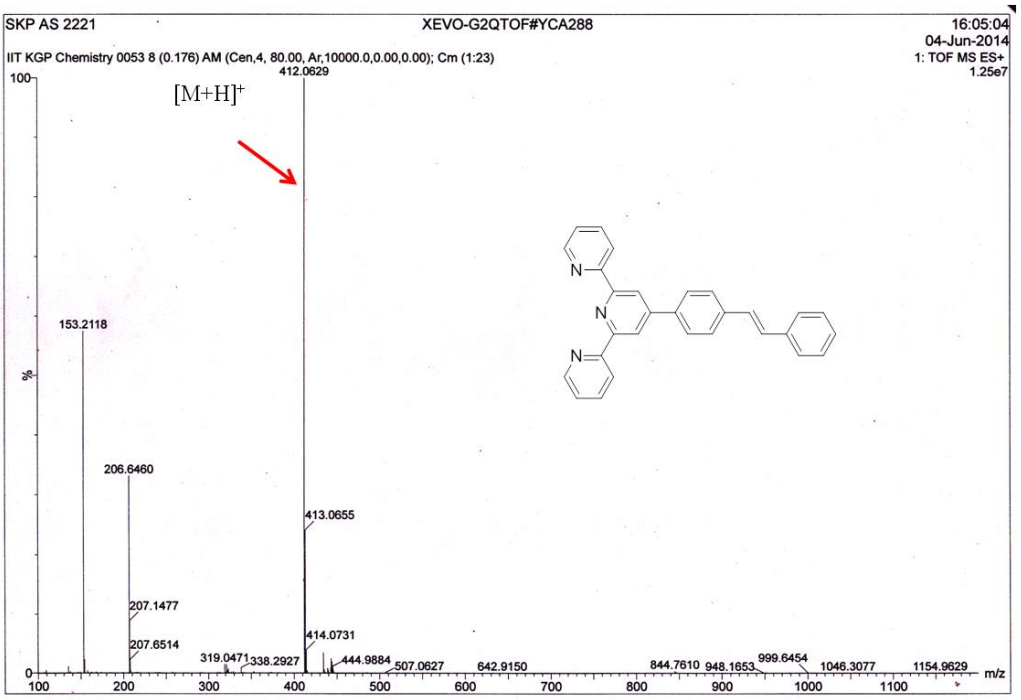

Fig. S49: HRMS (ESI$^+$) of **L1**

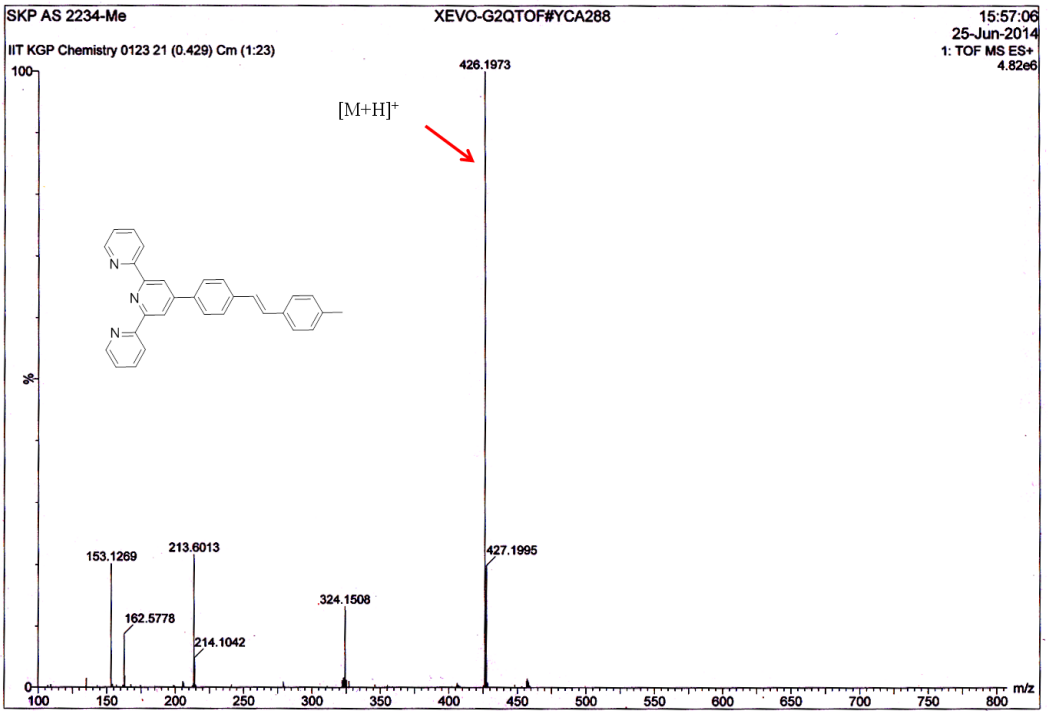

Fig. S50: HRMS (ESI$^+$) of **L2**

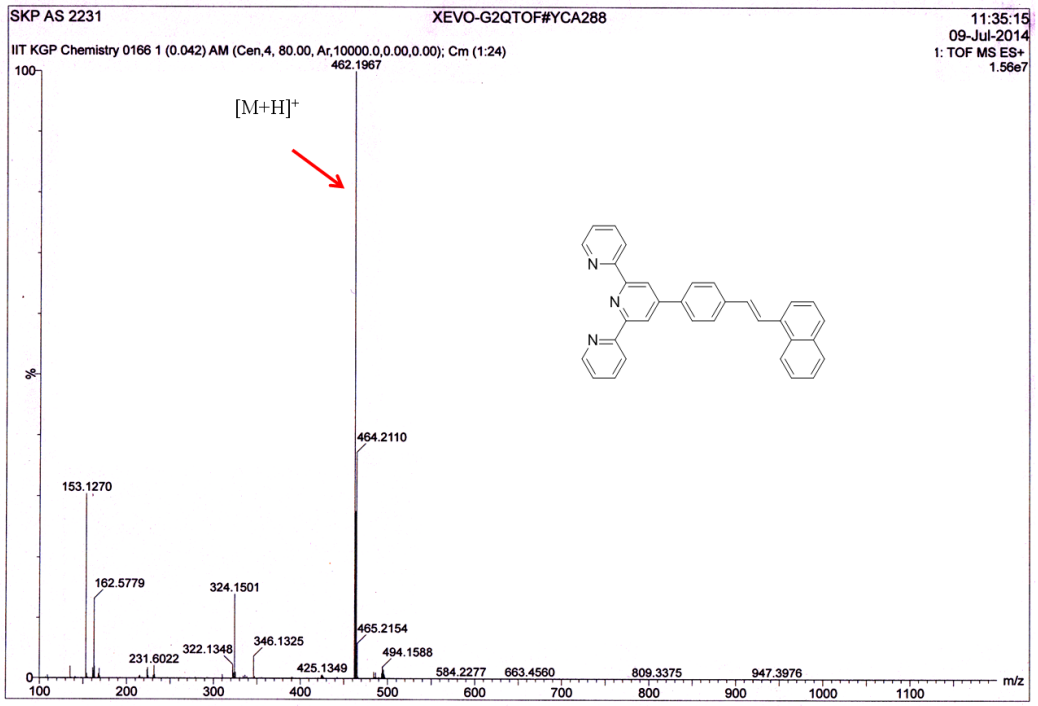

Fig. S51: HRMS (ESI^+) of **L3**

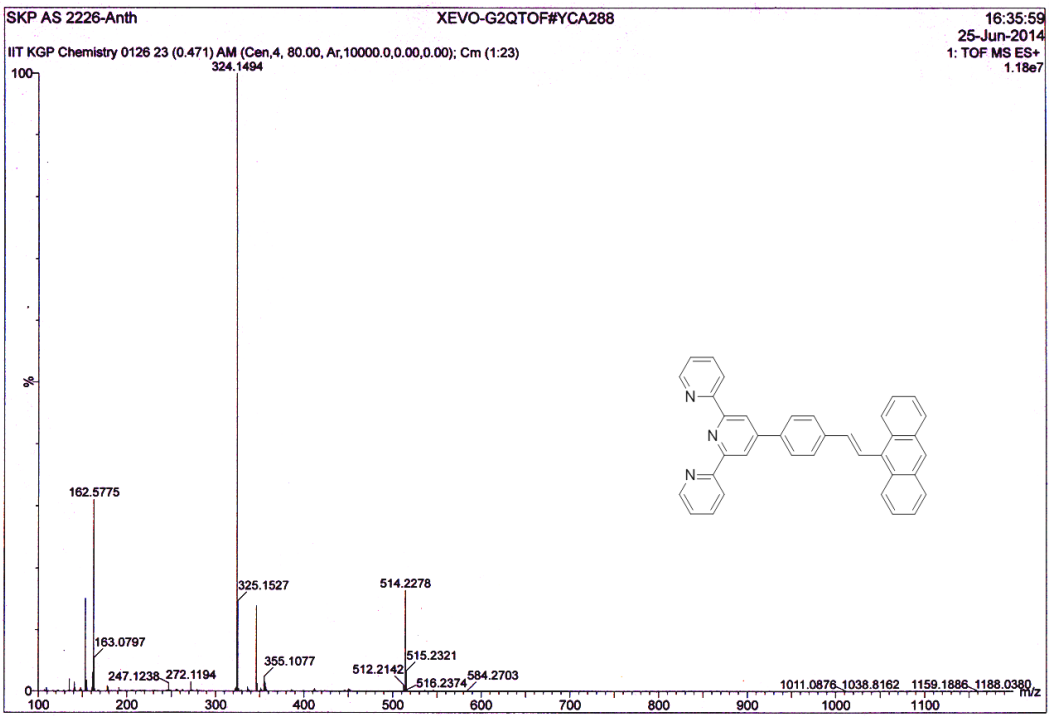

Fig. S52: HRMS (ESI^+) of **L4** (Interestingly, a peak was observed at 514.4276 corresponding to ($[M+3H]^+$) instead of 512.2126 for ($[M+H]^+$). However in LCMS study, the peak for ($[M+H]^+$) was observed as shown below.

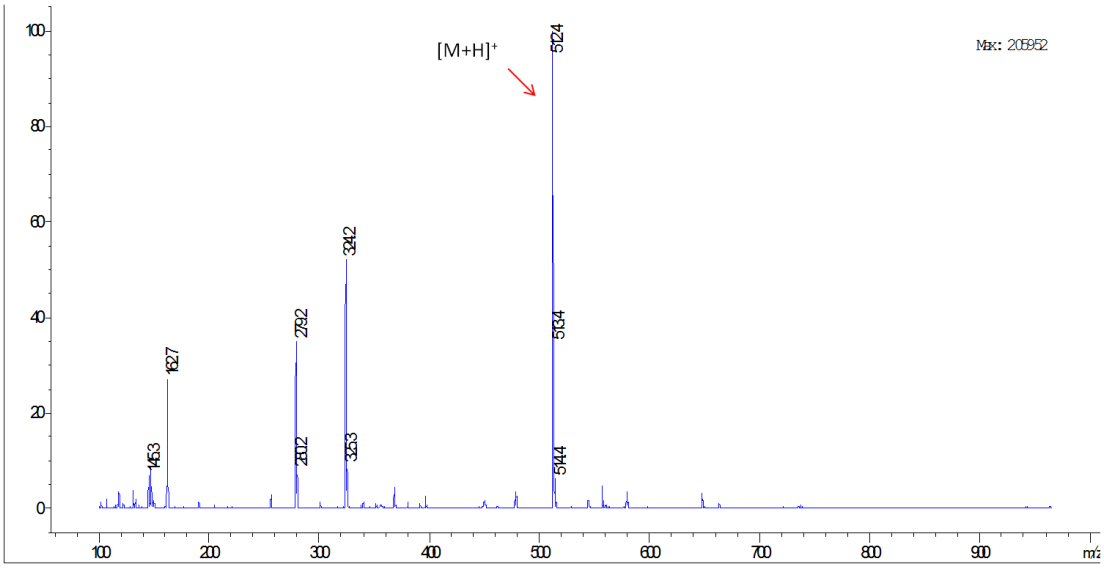

Fig. S53: LCMS (ESI^+) of **L4**; LCMS study was carried out in single quadruple mass analyzer (Agilent Technologies, A6120BW).

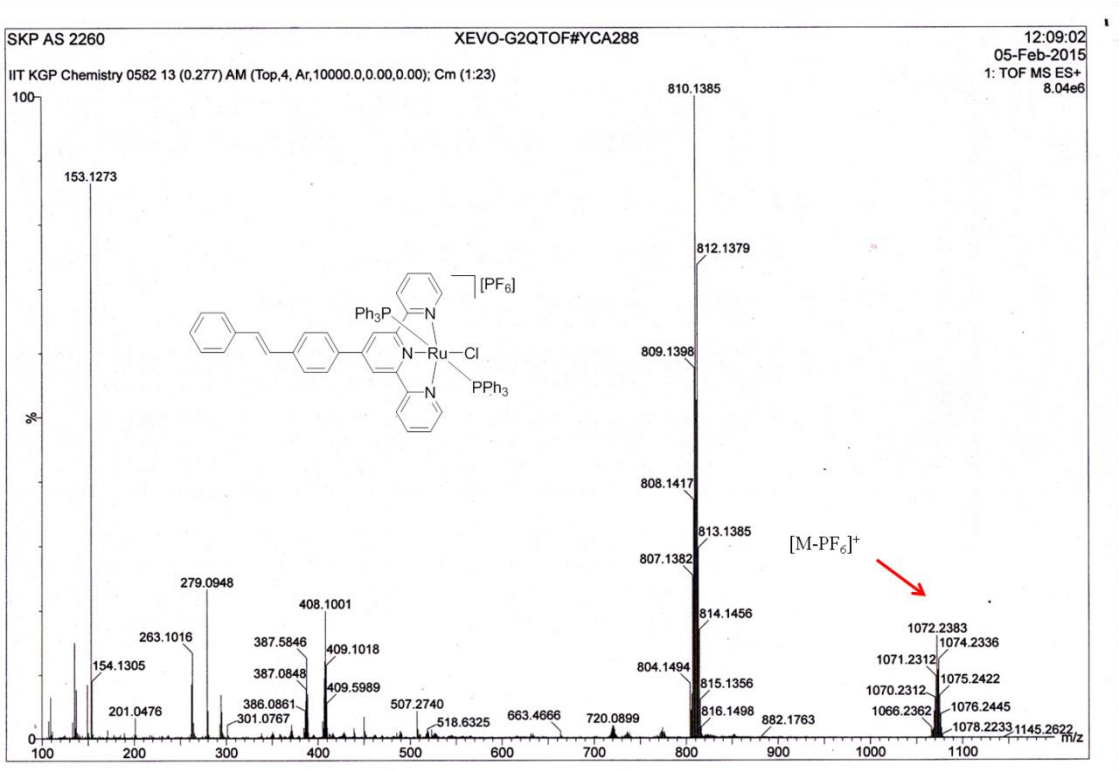

Fig. S54: HRMS (ESI^+) of **1**

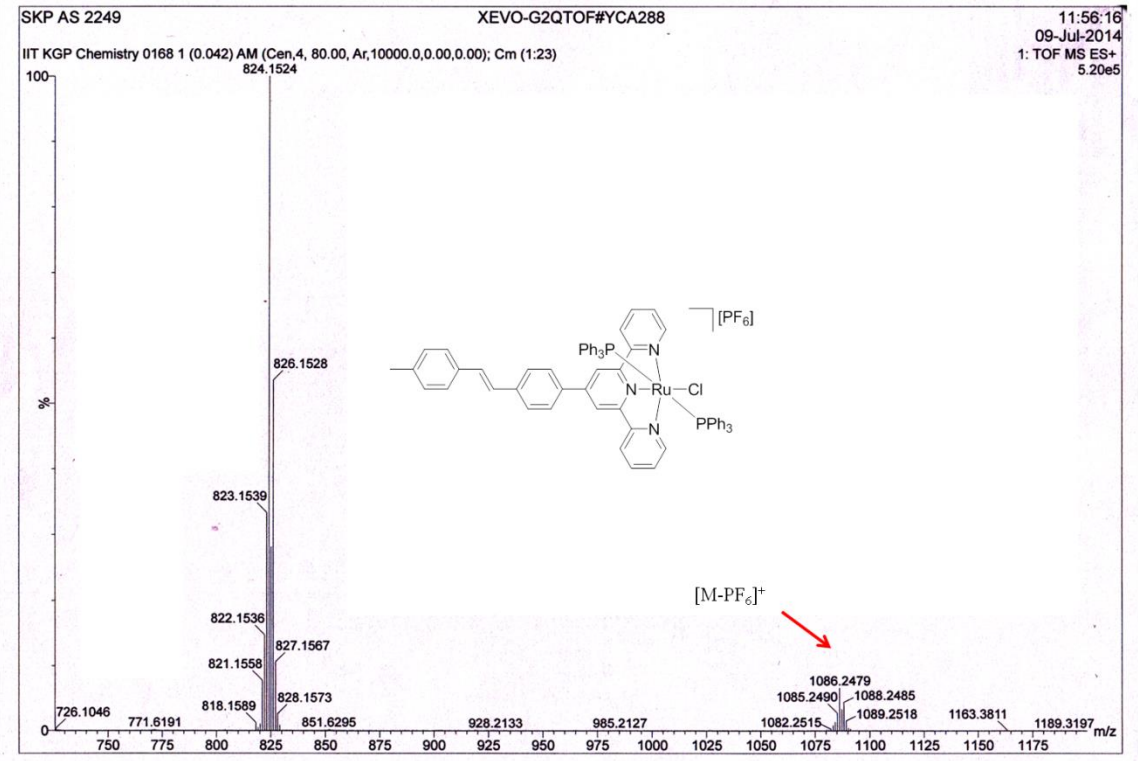

Fig. S55: HRMS (ESI$^+$) of **2**

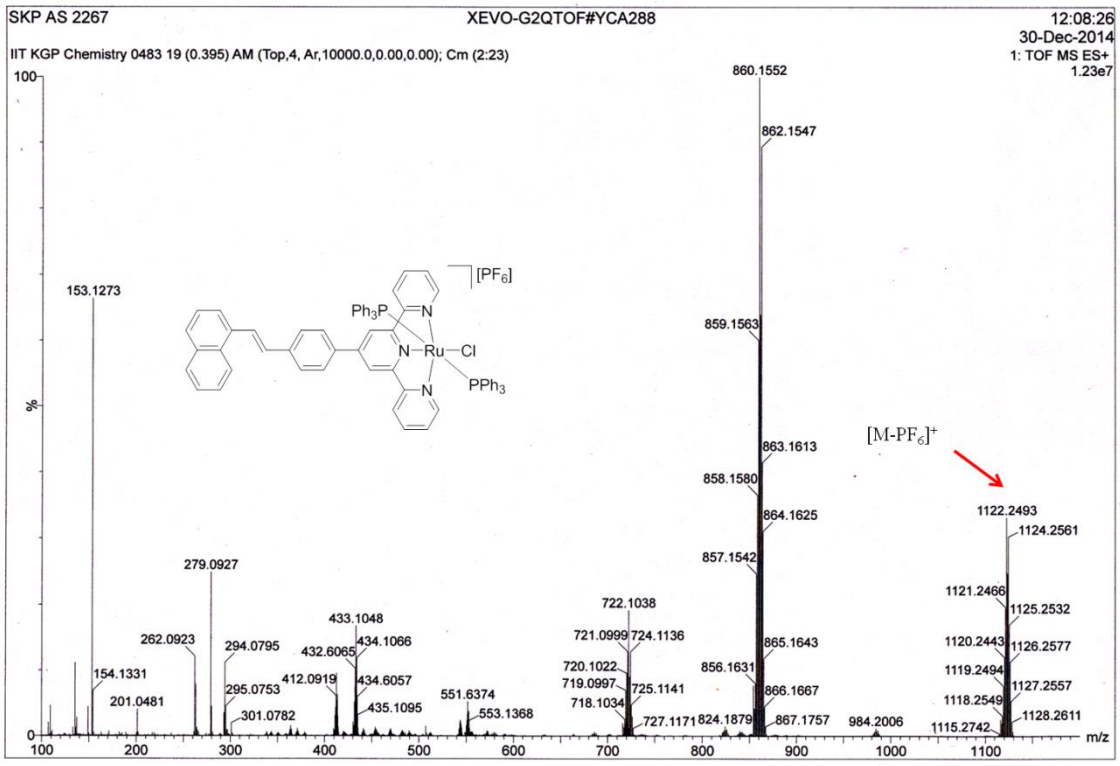

Fig. S56: HRMS (ESI$^+$) of **3**

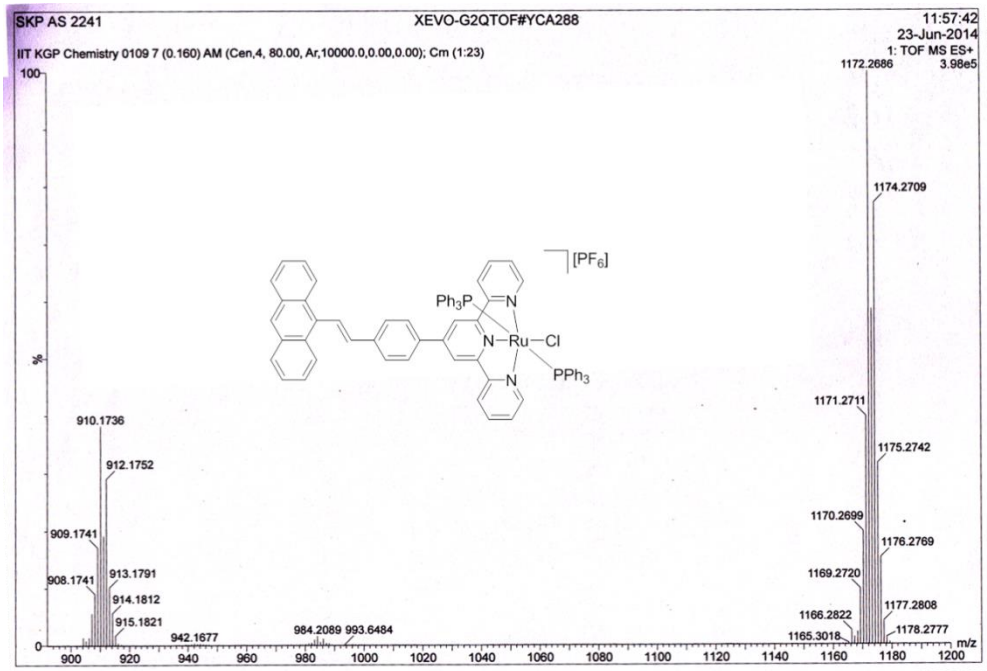

Fig. S57: HRMS (ESI$^+$) of **4**

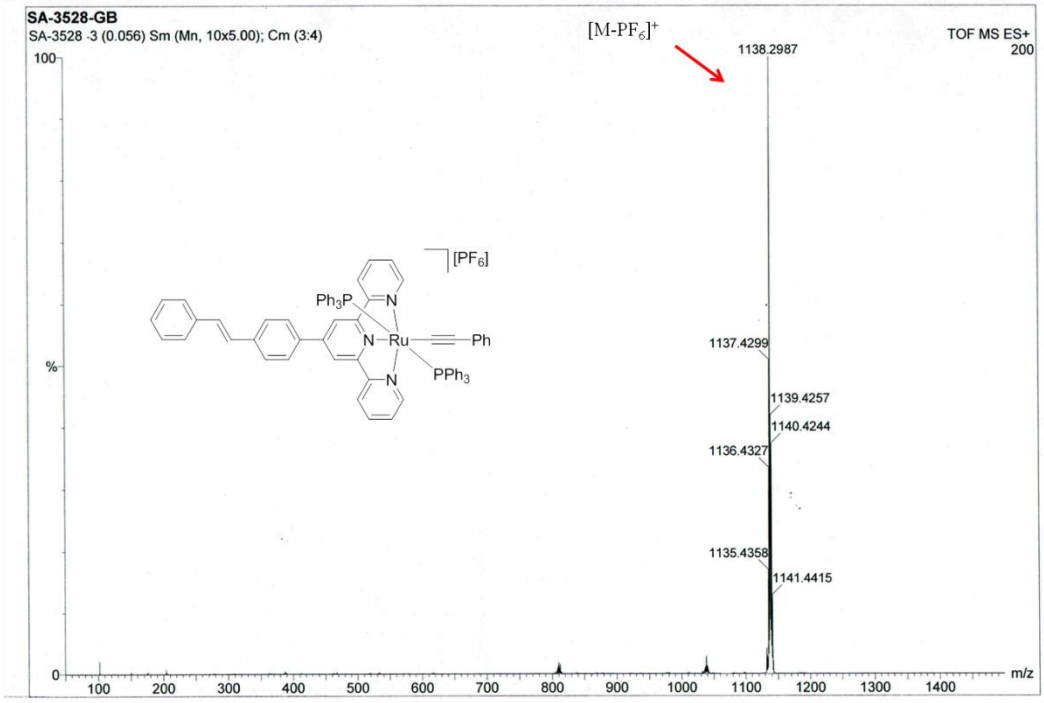

Fig. S58: HRMS (ESI$^+$) of **5**

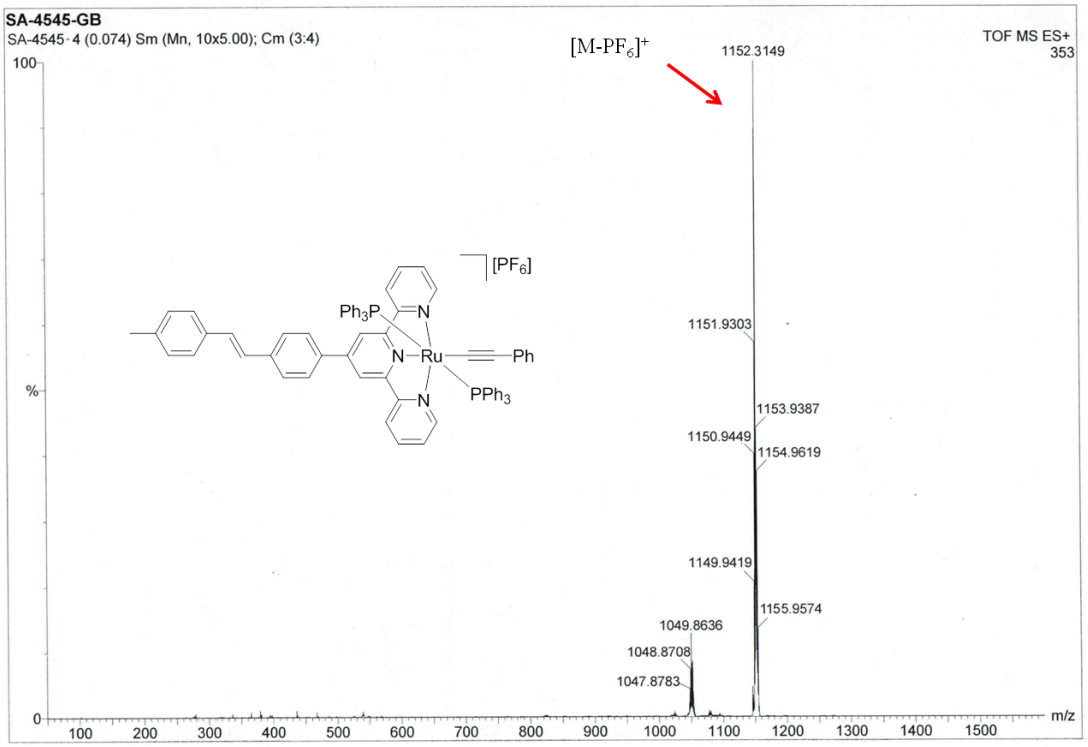

Fig. S59: HRMS (ESI$^+$) of **6**

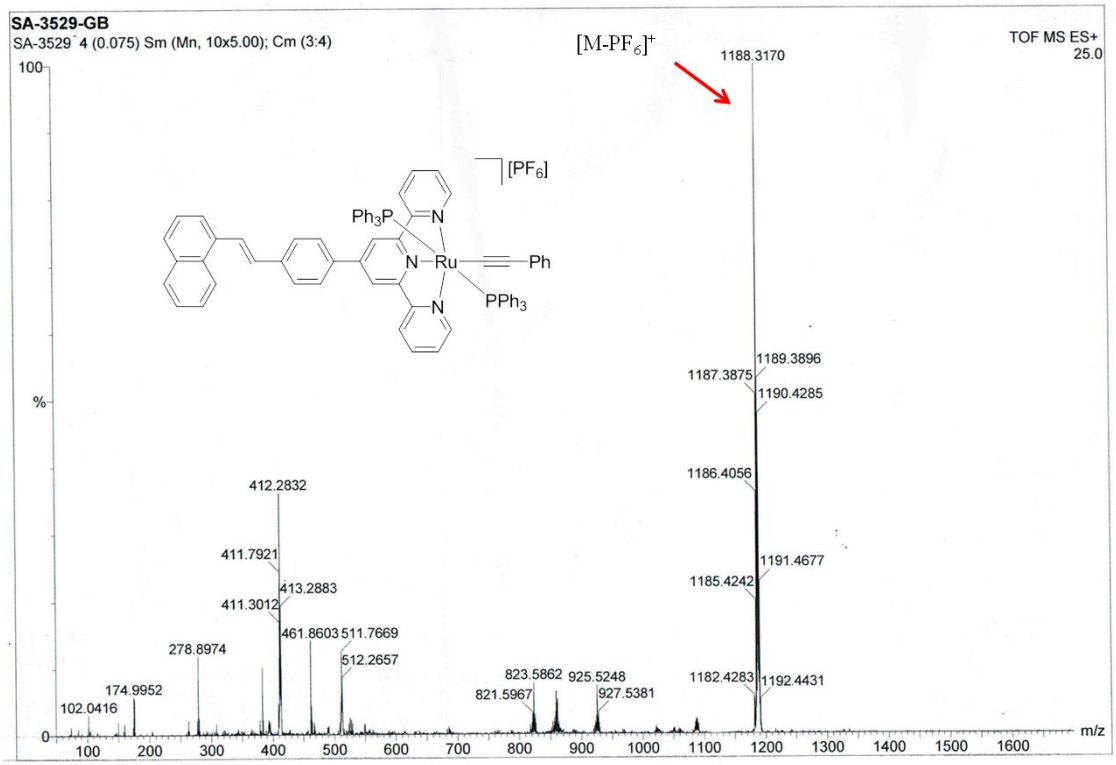

Fig. S60: HRMS (ESI$^+$) of **7**

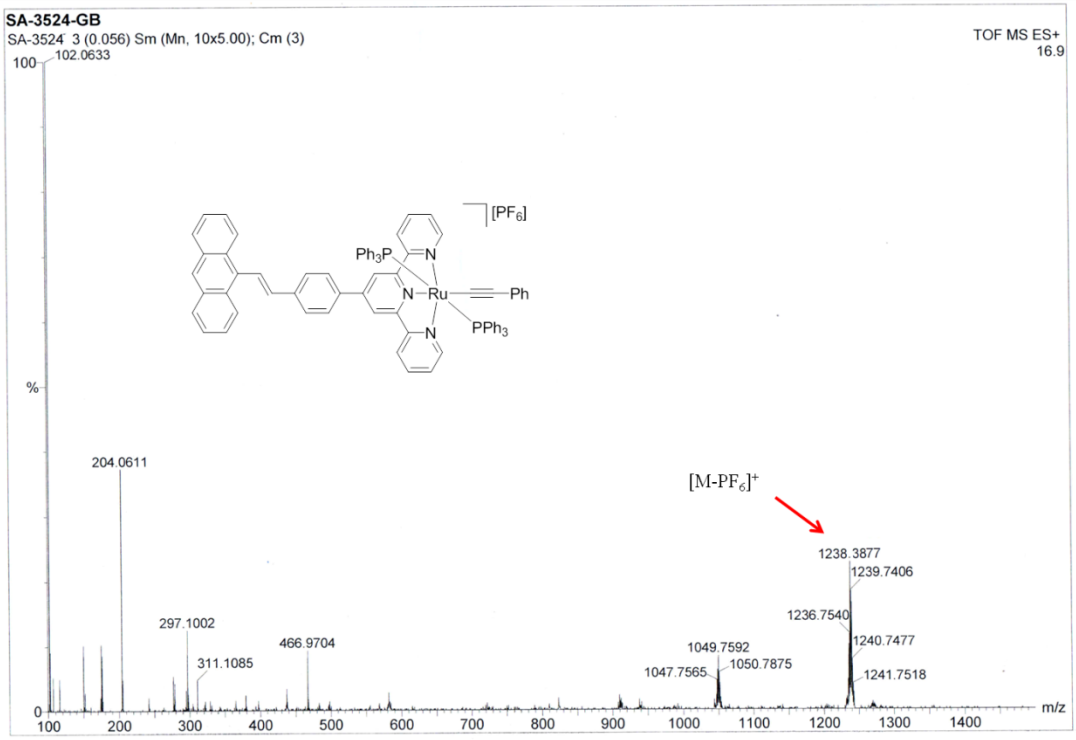

Fig. S61: HRMS (ESI^+) of **8**

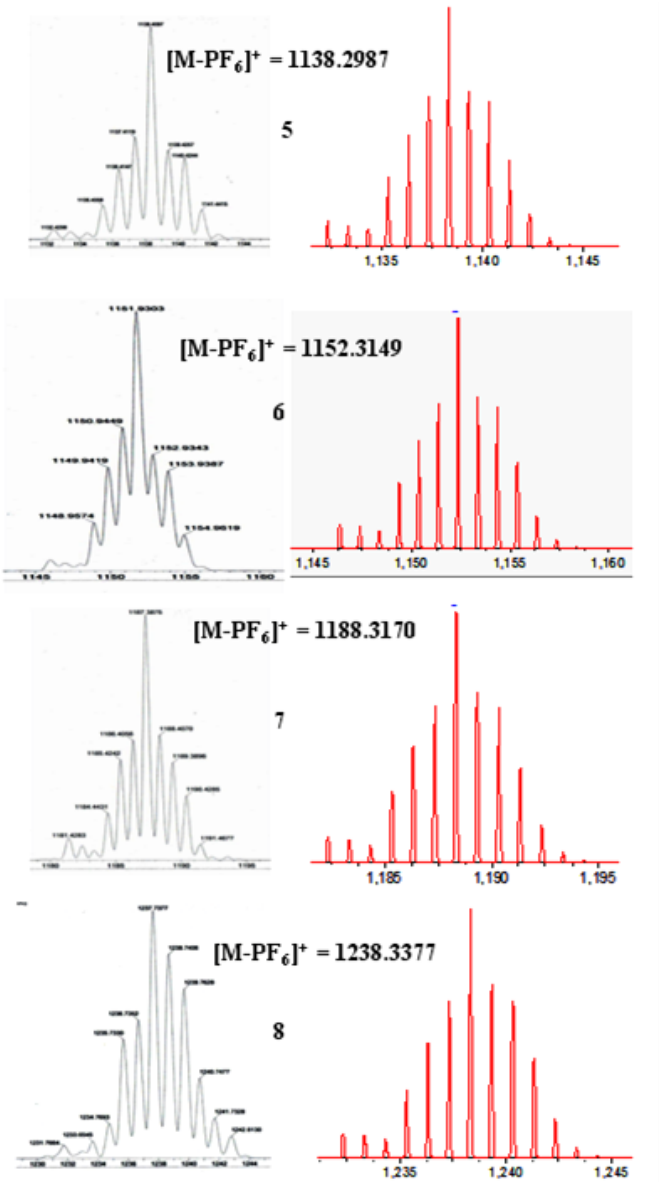

Fig. S62: Simulated and isotopic distribution pattern for the molecular ion peaks ($[M\text{-}PF_6]^+$) of complex **5-8** obtained from HRMS (ESI+).

2. Crystallographic data and refinement parameters

Table S1. Crystallographic data and refinement parameters for complex **1', 1, 2, 3'** and **3.**

	Complex 1'	**Complex 1**	**Complex 2**	**Complex 3'**	**Complex 3**
Empirical formula	$C_{94}H_{72}Cl_2F_{12}N_6P_4Ru_2$	$C_{65}H_{49}ClF_7N_3P_3Ru$	$C_{66.50}H_{52}Cl_{1.75}F_6N_3P_3Ru$	$C_{102}H_{76}Cl_2F_{12}N_6P_4Ru_2$	$C_{69}H_{0.25}ClF_7N_3P_3Ru$
Formula weight	1910.49	1234.50	1263.13	2010.60	1233.40
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Monoclinic
Space group	*P*$\bar{1}$	*P*$\bar{1}$	*P*$\bar{1}$	*P*$\bar{1}$	P21/c
a, Å	13.050(2)	14.204(3)	14.302(3)	13.293(4)	14.489(4)
b, Å	13.456(2)	17.591(3)	17.622(4)	13.425(4)	17.629(5)
c, Å	15.248(2)	22.635(4)	22.401(5)	14.198(4)	23.036(7)
α, deg	70.943(4)	89.925(7)	90	91.251(9)	90
β, deg	68.971(4)	81.885(6)	81.923(8)	95.993(9)	97.774(8)
γ, deg	61.317(4)	89.877(6)	90	115.779(8)	90
V, Å^3	2153.3(6)	5599.1(19)	5590(2)	2262.7(10)	5830(3)
Z	1	4	4	1	4
ρ_{calcd}, g cm^{-3}	1.473	1.464	1.501	1.476	1.405
μ, mm^{-1}	0.564	0.482	0.517	0.541	0.464
F(000)	968	2516	2579	1296	2417
Collected	25533	71643	66071	26317	47182
independent	8665	21934	19515	7861	6327
Observed [I > 2σ(I)]	4294	14058	9841	3607	5121
No. of variables	541	1449	1479	577	761
Goodness-of-fit	1.032	1.046	0.988	0.968	1.055
Final R indices [I>2σ(I)][a]	R1=0.1079	R1= 0.0615	0.0763	R1= 0.0991	R1= 0.0584
	wR2= 0.2849	wR2= 0.1478	0.1797	wR2=0.2395	wR2= 0.1535
R indices (all data)[a]	R1=0.2263	R1= 0.1047	0.1572	R1=0.2014	R1= 0.0727
	wR2=0.3584	wR2= 0.1726	0.2306	wR2=0.3068	wR2=0.1661

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ with $F_o^2 > 2\sigma(F_o^2)$. $wR_2 = [\Sigma w(|F_o^2| - |F_c^2|)^2/\Sigma|F_o^2|^2]$; Data was collected at 100 K for the single crystals of complex **1**, **1′**, **2**, **3′** whereas for complex **3** data was collected at 293(2) K.

3. Photophysical studies

3a. Determination of Quantum yield

All the UV−Vis absorption and fluorescence emission spectra were collected using a Shimadzu UV−Vis spectrophotometer (model UV 2450 and a Spex Fluorolog-3 spectrofluorimeter (model FL3−11) respectively. Throughout all the measurements, the concentration were maintained at (1×10^{-5} M). Fluorescence quantum yields were measured with respect to a secondary standard quinine sulphate (λ_{abs} = 350 nm) in 0.1 M H_2SO_4 (Φ = 0.54) at 298 K. The following equation was used to calculate the quantum yields[1]:

$$\frac{\boldsymbol{\Phi_S}}{\boldsymbol{\Phi_R}} = \frac{\boldsymbol{A_S}}{\boldsymbol{A_R}} \times \frac{(\boldsymbol{Abs})_{\boldsymbol{R}}}{(\boldsymbol{Abs})_{\boldsymbol{S}}} \times \frac{\boldsymbol{\eta_S^2}}{\boldsymbol{\eta_R^2}}$$

Here Φ represents the quantum yield, (Abs) represents the absorbance, A represents the area under the fluorescence curve, and η is the refractive index of the medium. The subscript S and R denote the corresponding parameters for the sample and reference respectively.

3b. Determination of time resolved fluorescence spectra

The time-resolved emission decays were recorded using a time correlated single photon counting (TCSPC) picoseconds spectrophotometer. **L1**, **L2** and **L3** were excited using a picosecond diode laser at 340 nm (IBH, UK, Nanoled) whereas **L4** were excited at 400 nm using the same laser, and the signals were recorded at magic angle (54.71) using a Hamamatsu micro channel plate photomultiplier tube (3809U). The typical instrument response function in our setup is 100 ps. The instrument response function of our setup is ~800 ps. Time-resolved fluorescence decays were analyzed using IBH DAS-6 decay analysis software.

3c. Photophysical data of the ligands

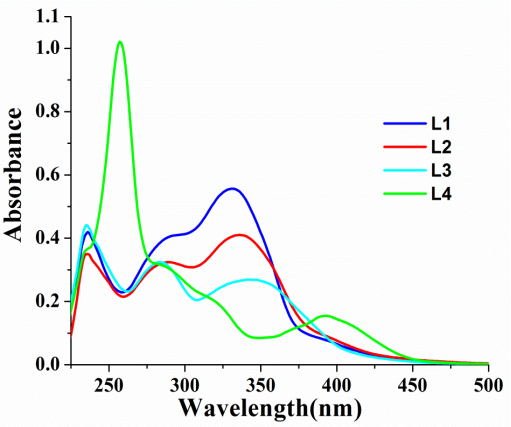

Fig. S63: (a) Absorption spectra of **L1-L4** in 1×10^{-5} M $CHCl_3$ solution at ambient temperature.

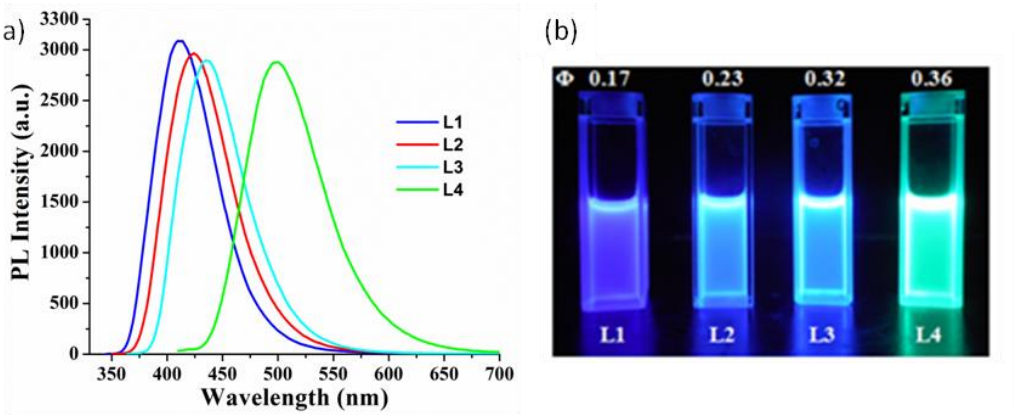

Fig. S64: (a) Emission spectra of **L1-L4** in 1×10^{-5} M $CHCl_3$ solution at ambient temperature. (b) Visual appearance of **L1-L4** in $CHCl_3$ (1×10^{-4} M) under UV illumination at 365 nm.

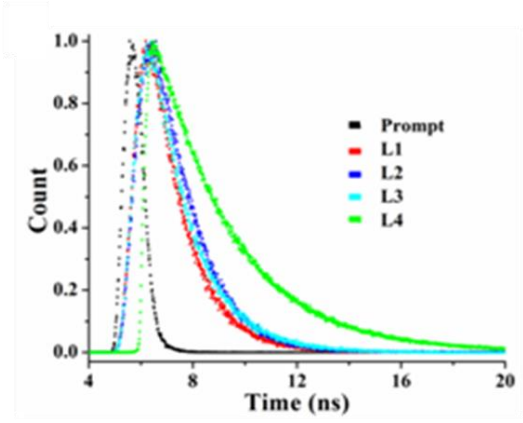

Fig. S65: Time resolved fluorescence spectra of **L1-L4**

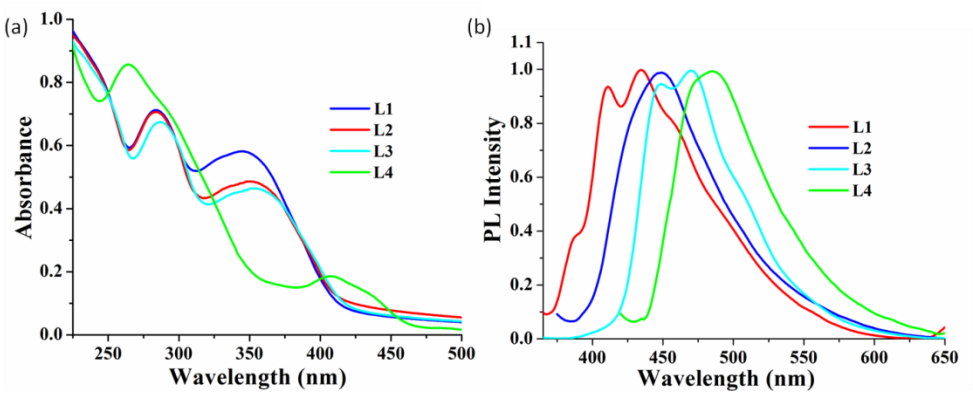

Fig. S66: Solid state (a) absorption and (b) emission spectra of **L1-L4** at ambient temperature.

Table S2. Photophysical data of the arylene-vinylene conjugated terpyridines chloroform thin films at 28 °C.

Ligands	Absorption (nm) [ε ($M^{-1}.cm^{-1}$)×10^4]	Emission (λ_{ex}) (nm)	Stokes Shift (cm^{-1})	Lifetime (ns)	Q. Y.* (%)
L1	333(4.1), 288(3.2)	412(333)	5758.2	1.33	17
L2	334(4.8), 285(3.1)	417(334)	1666.7	1.36	23
L3	341(5.6), 284(5.0)	437(341)	1552.8	1.91	32
L4	390(1.0),258(9.0)	498(390)	1798.6	2.88	36

*Quinine sulphate (0.1 M H_2SO_4; Φ = 0.54) was used as reference for quantum yield calculation; ε =Absorption coefficient. Stokes shifts $\Delta\lambda_{st}$, cm^{-1} = λ_{em} - λ_{abs}.

Table S3: Photophysical data of the arylene-vinylene conjugated terpyridines in thin films at 28 °C.

Ligands	Absorption (nm)	Emission (nm)	[a]Stokes Shift (cm^{-1})
L1	346, 284	435,415 (sh)	5913
L2	354,285	440	5521
L3	357, 286	470, 448	6177
L4	408, 263	504	4668

[a]Stokes shifts $\Delta\lambda_{st}$, cm^{-1} = λ_{em} - λ_{abs}.

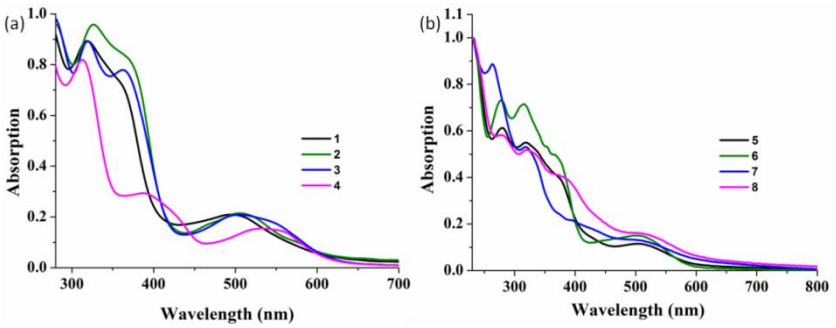

Fig. S67: Solid state absorption spectra of complex **1-8** at ambient temperature.

4. Electrochemical Characterization

Cyclic voltammetric analysis was conducted in acetonitrile using n-Bu_4NPF_6 (0.1 M) as supporting electrolytes, Pt wire counter electrode and Ag/AgCl reference electrode.

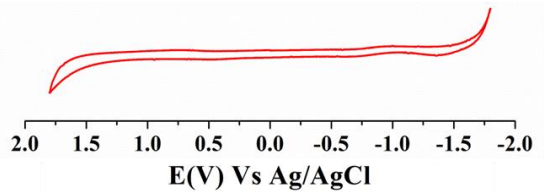

Fig. S68: Cyclic voltammogram of acetonitrile using $TBAPF_6$ as supporting electrolyte (Blank run), Pt disc working electrode, and Ag/AgCl reference electrode. Scan rate at 100mV/s.

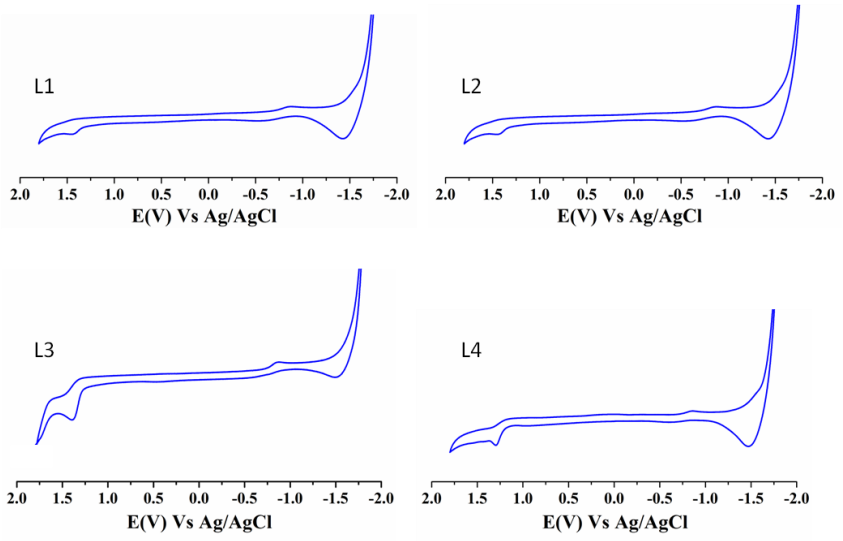

Fig. S69: Cyclic voltammogram of the free ligands (**L1-L4)** in acetonitrile using $TBAPF_6$ as supporting electrolyte, Pt disc working electrode, and Ag/AgCl reference electrode. Scan rate at 100 mV/s.

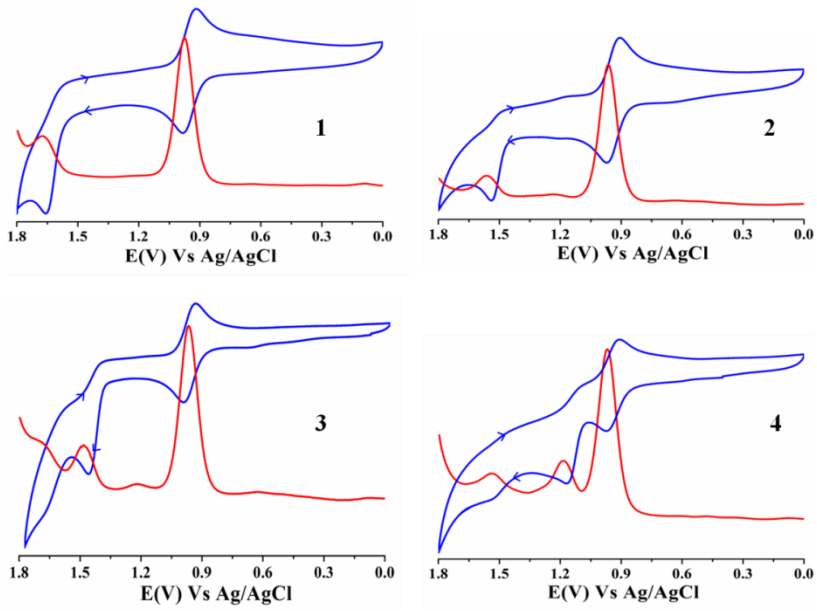

Fig. S70: Cyclic voltammograms (CV) and differential pulse voltammograms (DPV) of ruthenium(II) complexes (**1-4**) in acetonotrile solution using $TBAPF_6$ as supporting electrolyte, Pt disc working electrode, and Ag/AgCl reference electrode. Scan rate at 100 mV/s.

Table S4. Electrochemical data for complexes **1-4** in acetonitrile.

complex	anodic		cathodic
	[b]E_{pa} (V)	[c]$E_{1/2}$ (V)	[b]E_{pc} (V)
1	1.65	0.93 (65)	-1.38, -1.54
2	1.52	0.93(60)	-1.32, -1.51
3	1.68, 1.46	0.94(84)	-1.38, 1.53
4	1.54, 1.17	0.94(62)	-1.33, -1.55

[a]condition: Pt-disc working electrode, Ag/AgCl reference electrode, Pt wire counter electrode, 0.1 M $TBAPF_6$ in acetonitrile, scan rate 100 mV s^{-1} at 25 ˚C. [b]irreversible redox waves. [c]reversible redox waves. [c] reversible redox waves and corresponding E_{pa}-E_{pc} values in parenthesis.

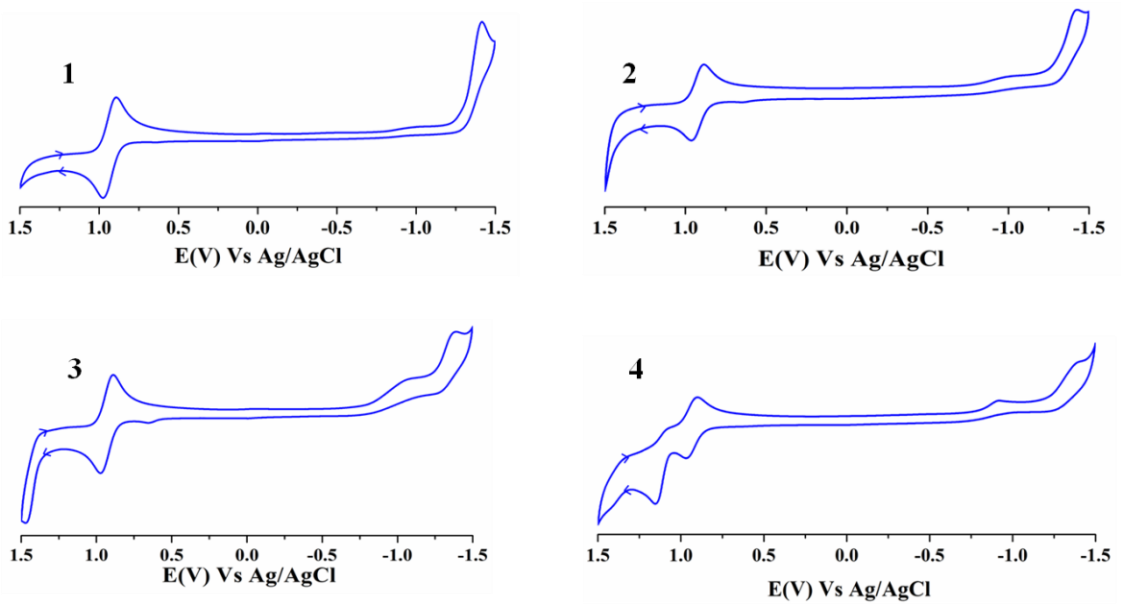

Fig. S71: Cyclic voltammogram of complex **1-4** in DCM solution using $TBAPF_6$ as supporting electrolyte, Pt disc working electrode, and Ag/AgCl reference electrode. Scan rate at 100 mV/s.

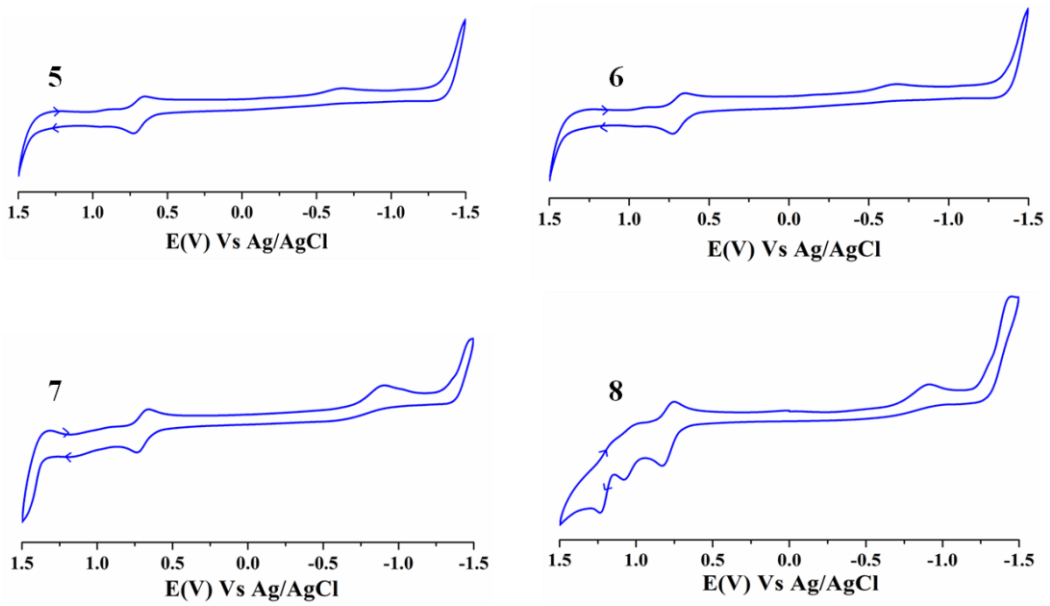

Fig. S72: Cyclic voltammogram of complex **5-8** in DCM solution using $TBAPF_6$ as supporting electrolyte, Pt disc working electrode, and Ag/AgCl reference electrode. Scan rate at 100 mV/s.

5. Theoretical studies for the complexes 1-8.

The DFT study of all the Ru(II) complexes were analyzed using CAM-B3LYP/ DEF2-TZVP basis set in conjunction of polarization continium model (PCM) together with dichloromethane as solvent.

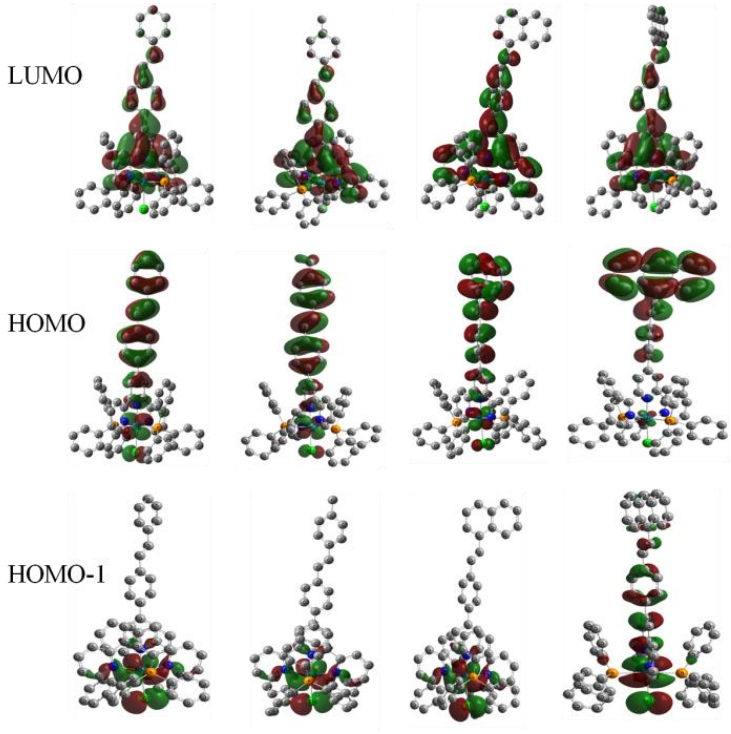

Fig. S73: Frontier molecular orbitals of the Ru(II) complexes (**1-4**) estimated by DFT calculations using CAM-B3LYP functional and def2-TZVP basis set.

Table S5: The HOMO-LUMO gap in the complexes **1-8** together with the Ru d-orbital ontributions (in %) in the HOMO , HOMO-1and LUMO, LUMO+1.

Complex	E_{HOMO}/E_{LUMO} (eV)	Bandgap (eV)	Ru d-orbital contribution in HOMO (%)	Ru d-orbital contribution in HOMO-1 (%)	Ru d-orbital contribution in LUMO (%)	Ru d-orbital contribution in LUMO+1 (%)
1	-7.32/-1.83	5.49	23.7	72.3	4.8	0.8
2	-7.23/-1.82	5.41	14.2	72.4	4.8	0.8
3	-7.22/-1.83	5.38	10.8	72.1	5.0	0.7
4	-6.84/-1.83	5.01	0.7	57.9	4.7	0.7
5	-6.73/-1.75	4.97	37.9	45.9	4.4	0.8
6	-6.72/-1.74	4.97	37.9	40.2	4.4	0.8
7	-6.73/-1.75	4.97	37.8	41.4	4.4	0.8
8	-6.74/-1.76	4.98	37.4	2.6	3.9	0.8

Table S6: Computational result of optimized structure of complex **1**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.01107	0.11129	0.02347
Cl	0.1379	0.5309	2.50909
P	2.46431	0.04766	0.06579
P	-2.47848	0.1258	0.14294
N	-0.11913	-2.02328	-0.24736
C	0.02738	2.32014	-1.90129
C	0.67767	0.59378	-6.99182
H	-1.22643	1.40835	-6.52988
C	0.0239	0.9989	-4.08516
H	0.12106	1.89622	-4.68208
N	-0.06431	-0.0482	-1.96362
C	0.02358	-0.55736	-9.00839
N	0.01359	2.15159	-0.55134
C	-3.30323	-2.35181	3.33347
H	-2.7592	-2.75385	4.18215
C	-0.06032	-0.24655	-4.71459
C	3.27354	1.50962	0.83499
C	0.00321	1.07471	-2.70106
C	-0.20737	-2.37596	-1.55876
C	-0.03572	-0.35626	-6.18854
C	-0.14126	-2.98848	0.67723
H	-0.06383	-2.66192	1.7046
C	0.00646	3.22705	0.24016
H	0.02152	3.02157	1.30293
C	3.7191	3.8949	0.84814
H	3.5994	4.86841	0.384
C	0.0933	-0.71489	-10.46534
H	0.67918	-1.56921	-10.79558
C	-2.64087	-1.54274	2.41302
H	-1.60052	-1.28576	2.56701
C	-3.3233	-1.01358	1.3181
C	0.03759	3.58924	-2.46511
H	0.04965	3.71122	-3.54058
C	0.00344	4.52124	-0.2622
H	-0.00585	5.36121	0.42159
C	-0.32193	-3.70586	-1.94332
H	-0.39332	-3.96699	-2.99109
C	3.25532	-0.10657	-1.59565
C	-5.10623	3.32608	0.38422
H	-6.0084	3.66656	-0.11368
C	3.22967	-1.36433	0.96764
C	-0.16575	-1.3858	-3.91271
H	-0.26257	-2.35886	-4.37578
C	0.63633	-1.40832	-6.81574
H	1.1672	-2.14405	-6.22008
C	-3.92953	-2.07337	-3.02678
H	-4.1915	-3.10985	-3.21279
C	4.59679	2.50851	2.60203

H	5.16676	2.3934	3.51815
C	4.44611	-1.9192	0.55449
H	4.94418	-1.54588	-0.3323
C	-0.41585	-0.07676	-12.83901
C	-0.65045	0.49503	-8.37206
H	-1.16502	1.24772	-8.95878
C	-1.15199	0.68938	-15.02444
H	-1.75067	1.36895	-15.62244
C	4.01495	1.39057	2.01331
H	4.1422	0.42229	2.48126
C	-0.36308	-0.27486	-15.64124
C	-4.58602	4.04359	1.45551
H	-5.07771	4.94969	1.79453
C	5.03233	-2.9532	1.27489
H	5.97454	-3.37346	0.93846
C	-3.43939	3.58762	2.09684
H	-3.03406	4.13319	2.94298
C	-0.1539	-1.26119	-2.53147
C	-3.17873	-0.35796	-1.48591
C	-3.51195	-1.68901	-1.75655
H	-3.45618	-2.4347	-0.97149
C	0.02307	4.70457	-1.63576
H	0.02681	5.70059	-2.06363
C	0.66543	-1.50232	-8.19825
H	1.2037	-2.32151	-8.6652
C	4.45339	3.76277	2.02161
H	4.91099	4.63318	2.48025
C	3.12856	2.78018	0.26523
H	2.56474	2.90907	-0.6508
C	-1.17524	0.78612	-13.63854
H	-1.79359	1.5414	-13.16193
C	4.34775	-0.48145	-4.15542
H	4.76991	-0.62506	-5.14456
C	4.41804	-3.44326	2.4226
H	4.87707	-4.25071	2.98392
C	4.04646	0.8808	-2.18584
H	4.26928	1.79667	-1.6545
C	-0.25534	-4.33408	0.35996
H	-0.26938	-5.07177	1.15287
C	-5.34692	-2.09679	2.09086
H	-6.40458	-2.30352	1.96384
C	-0.48749	0.07328	-11.37996
H	-1.08742	0.91723	-11.0468
C	3.03681	-1.2945	-2.30561
H	2.4643	-2.09774	-1.85424
C	4.58419	0.69517	-3.45705
H	5.19859	1.47519	-3.89474
C	-0.34876	-4.69892	-0.97404
H	-0.44013	-5.74023	-1.26114
C	-4.68968	-1.28746	1.17489
H	-5.2461	-0.86967	0.34266
C	-2.80692	2.42931	1.65988

H	-1.92371	2.06698	2.17587
C	3.5773	-1.48204	-3.57037
H	3.40105	-2.41415	-4.09758
C	-3.31412	1.71003	0.57264
C	-3.67097	0.18801	-3.79757
H	-3.72919	0.92669	-4.59047
C	-3.25112	0.57237	-2.53
H	-2.98958	1.6106	-2.35406
C	0.40241	-1.13795	-14.85976
H	1.02494	-1.89035	-15.33346
C	-4.65258	-2.63605	3.17127
H	-5.16776	-3.26751	3.88795
C	-4.0137	-1.13667	-4.04967
H	-4.34363	-1.43569	-5.03909
C	3.21862	-2.88673	2.85149
H	2.73889	-3.25314	3.75345
C	-4.48006	2.16291	-0.05164
H	-4.91228	1.61191	-0.87831
C	0.37853	-1.04048	-13.47633
H	0.98964	-1.71748	-12.88907
C	2.62729	-1.85437	2.13013
H	1.70958	-1.40006	2.48501
H	-0.3406	-0.35359	-16.72324

Table S7: Computational result of optimized structure of complex **2**

Atoms	**Coordinates (Angstroms)**		
	X	**Y**	**Z**
Ru	-0.01027	0.11982	0.03058
Cl	0.14462	0.58175	2.50858
P	2.46541	0.06787	0.06522
P	-2.47696	0.12296	0.15779
N	-0.10756	-2.01933	-0.20735
C	0.01015	2.29874	-1.92822
C	-0.70934	0.48278	-6.98983
H	-1.26492	1.299	-6.53901
C	0.00633	0.94425	-4.09175
H	0.095	1.833	-4.7028
N	-0.06827	-0.07072	-1.95399
C	-0.00946	-0.69813	-8.99014
N	0.00157	2.15088	-0.57577
C	-3.27759	-2.30575	3.39163
H	-2.72843	-2.69127	4.24466
C	-0.07135	-0.31137	-4.7016
C	3.27304	1.54661	0.80369
C	-0.00995	1.0411	-2.70884
C	-0.19659	-2.39278	-1.51294
C	-0.05172	-0.44508	-6.17345
C	-0.12232	-2.97024	0.73212
H	-0.04468	-2.62757	1.75419
C	-0.00814	3.23825	0.19929
H	0.01087	3.04891	1.26499

C	3.70933	3.93349	0.77358
H	3.58234	4.89857	0.29405
C	0.04994	-0.88391	-10.44394
H	0.62637	-1.74941	-10.76149
C	-2.62265	-1.50882	2.45542
H	-1.58303	-1.24414	2.60093
C	-3.3119	-1.00084	1.35479
C	0.01333	3.55916	-2.51119
H	0.02205	3.66488	-3.58837
C	-0.01845	4.5246	-0.32271
H	-0.02944	5.37491	0.34813
C	-0.30433	-3.72918	-1.8766
H	-0.37629	-4.00735	-2.91997
C	3.24933	-0.11556	-1.59679
C	-5.12183	3.31212	0.3503
H	-6.02699	3.63871	-0.15146
C	3.24	-1.3242	0.98996
C	-0.16662	-1.43874	-3.88182
H	-0.25825	-2.41929	-4.32979
C	0.62839	-1.50067	-6.78596
H	1.1715	-2.2193	-6.18048
C	-3.9277	-2.13628	-2.96971
H	-4.18585	-3.17685	-3.13727
C	4.60535	2.58026	2.5439
H	5.18247	2.48268	3.45758
C	4.45987	-1.87798	0.58534
H	4.95487	-1.51635	-0.30801
C	-0.46877	-0.28306	-12.82563
C	-0.69144	0.35797	-8.36813
H	-1.2218	1.0917	-8.96474
C	-1.08714	0.53449	-15.02893
H	-1.59369	1.27836	-15.63713
C	4.02359	1.4504	1.97835
H	4.15838	0.4906	2.46138
C	-0.42161	-0.52093	-15.6491
C	-4.60313	4.05144	1.40738
H	-5.099	4.96073	1.73143
C	5.05332	-2.89573	1.3227
H	5.99808	-3.31542	0.99278
C	-3.4525	3.61327	2.05398
H	-3.04832	4.17607	2.88932
C	-0.15191	-1.29282	-2.50276
C	-3.1798	-0.39168	-1.46057
C	-3.50821	-1.72852	-1.70741
H	-3.4473	-2.46042	-0.90982
C	-0.00357	4.68697	-1.69893
H	-0.00526	5.67636	-2.14196
C	0.64915	-1.62	-8.16659
H	1.19376	-2.44154	-8.62194
C	4.45288	3.824	1.94353
H	4.91053	4.70374	2.38394
C	3.11872	2.80692	0.21397

H	2.54743	2.91879	-0.6996
C	-1.11141	0.65062	-13.64447
H	-1.63679	1.48421	-13.18674
C	4.32817	-0.53452	-4.15542
H	4.74514	-0.69521	-5.14414
C	4.44295	-3.3703	2.47903
H	4.90765	-4.16509	3.05359
C	4.02395	0.86792	-2.21469
H	4.23933	1.7981	-1.70559
C	-0.22945	-4.3212	0.43604
H	-0.2377	-5.04657	1.24031
C	-5.32737	-2.08049	2.15321
H	-6.38456	-2.29409	2.03389
C	-0.52456	-0.10449	-11.37053
H	-1.0993	0.76166	-11.04982
C	3.0402	-1.32163	-2.27842
H	2.48055	-2.12119	-1.80485
C	4.55501	0.66031	-3.48528
H	5.1567	1.43768	-3.94481
C	-0.32344	-4.70717	-0.89195
H	-0.40937	-5.75334	-1.16257
C	-4.67752	-1.28325	1.2215
H	-5.2391	-0.88149	0.38485
C	-2.81452	2.45088	1.63624
H	-1.92811	2.10264	2.15644
C	3.57423	-1.53102	-3.54253
H	3.40565	-2.47686	-4.04736
C	-3.32018	1.7097	0.56306
C	-3.68102	0.1127	-3.7797
H	-3.74462	0.83745	-4.58494
C	-3.25914	0.5204	-2.52014
H	-3.00153	1.56256	-2.36264
C	0.22274	-1.45646	-14.83179
H	0.75176	-2.28756	-15.29016
C	-4.62623	-2.59879	3.23948
H	-5.13564	-3.22072	3.9685
C	-4.01874	-1.21755	-4.00819
H	4.35017	1.53482	4.9914
C	3.24024	2.81441	2.89939
H	2.76357	3.16855	3.80784
C	4.49003	2.14497	0.06629
H	4.92072	1.57699	0.88216
C	0.20128	1.34449	13.4519
H	0.71407	2.0929	12.85687
C	2.64176	1.79824	2.16109
H	1.72161	1.34364	2.50908
C	0.40467	0.66676	17.14714
H	0.6023	0.88477	17.51378
H	1.04974	1.49097	17.46945
H	0.75719	0.24199	17.63965

Table S8: Computational result of optimized structure of complex **3**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.03501	0.14382	0.04155
Cl	0.06301	0.87742	2.45259
P	2.44549	0.14343	0.09281
P	-2.49881	0.15057	0.29677
N	-0.03412	-2.01065	-0.01852
C	-0.13195	2.15125	-2.08214
C	-1.01543	-0.12306	-6.93472
H	-1.62458	0.66959	-6.51221
C	-0.19783	0.6257	-4.12801
H	-0.21084	1.46575	-4.8102
N	-0.10876	-0.21676	-1.91714
C	-0.30729	-1.38595	-8.88007
N	-0.06884	2.11332	-0.72301
C	-3.02394	-2.36644	3.5098
H	-2.47971	-2.59807	4.41983
C	-0.1944	-0.67763	-4.63583
C	3.21823	1.71679	0.64968
C	-0.15275	0.83382	-2.75823
C	-0.07003	-2.49731	-1.28962
C	-0.23377	-0.92365	-6.0934
C	-0.0036	-2.87748	0.9975
H	0.02257	-2.44398	1.98677
C	-0.03645	3.25741	-0.03514
H	0.01524	3.14756	1.04143
C	3.62393	4.08653	0.32088
H	3.49286	4.98045	-0.28008
C	-0.29766	-1.66473	-10.32105
H	0.22829	-2.57255	-10.60873
C	-2.49838	-1.44266	2.61224
H	-1.56387	-0.94007	2.83537
C	-3.18494	-1.12506	1.4359
C	-0.16804	3.36157	-2.76158
H	-0.2199	3.38213	-3.84247
C	-0.06692	4.4983	-0.65787
H	-0.03815	5.39906	-0.0571
C	-0.07305	-3.86357	-1.54016
H	-0.10027	-4.2335	-2.55676
C	3.25992	-0.22931	-1.52331
C	-3.63356	4.09017	0.70148
H	-3.55401	4.9933	0.10519
C	3.22897	-1.10857	1.19437
C	-0.14961	-1.73921	-3.72921
H	-0.17051	-2.75696	-4.09593
C	0.50627	-1.96193	-6.66455
H	1.14134	-2.58238	-6.04036
C	-3.95357	-1.74914	-3.03231
H	-3.81079	-2.72678	-3.48112
C	4.50327	2.98516	2.26573

H	5.0641	3.0144	3.19417
C	4.46446	-1.68549	0.87872
H	4.96751	-1.42875	-0.04589
C	-1.05721	-0.35385	-8.29894
H	-1.69544	0.26919	-8.91567
C	3.94738	1.78338	1.83993
H	4.08651	0.89543	2.444
C	-4.24165	4.12605	1.9515
H	-4.64102	5.05807	2.33775
C	5.06325	-2.59211	1.74547
H	6.02008	-3.03179	1.48338
C	-4.33427	2.96011	2.70173
H	-4.8065	2.9762	3.67852
C	-0.10765	-1.48132	-2.3666
C	-3.45332	-0.17697	-1.25004
C	-3.2852	-1.42731	-1.85903
H	-2.6518	-2.17473	-1.39491
C	-0.13526	4.55053	-2.04083
H	-0.16224	5.5015	-2.56057
C	0.46859	-2.18539	-8.03212
H	1.06134	-2.98937	-8.45761
C	4.34657	4.1391	1.50772
H	4.78457	5.07486	1.83918
C	3.05789	2.88878	-0.09916
H	2.49967	2.87419	-1.02791
C	4.39472	-0.94089	-3.99311
H	4.83384	-1.21423	-4.94688
C	4.44289	-2.93	2.94382
H	4.91209	-3.63782	3.61956
C	4.02672	0.68569	-2.24744
H	4.21625	1.67636	-1.85603
C	-0.00534	-4.25338	0.81565
H	0.02033	-4.90741	1.67858
C	-4.93516	-2.66962	2.08401
H	-5.88983	-3.14067	1.87357
C	-0.83724	-0.90368	-11.28276
H	-1.31113	0.03497	-11.00992
C	3.08921	-1.51539	-2.05226
H	2.54219	-2.26429	-1.49055
C	4.58469	0.3329	-3.47371
H	5.17971	1.05999	-4.01665
C	-0.04	-4.75482	-0.47546
H	-0.04193	-5.82329	-0.65828
C	-4.4155	-1.74265	1.1876
H	-4.97743	-1.50281	0.29295
C	-3.8267	1.76325	2.20704
H	-3.91337	0.86603	2.80722
C	3.65033	-1.86934	-3.27181
H	3.51065	-2.87503	-3.65528
C	-3.2114	1.71389	0.95352
C	-4.99527	0.41435	-3.02404
H	-5.67268	1.13779	-3.46598

C	-4.32871	0.73448	-1.84389
H	-4.51513	1.69636	-1.38483
C	-4.23945	-2.98725	3.24552
H	-4.64702	-3.71039	3.94461
C	-4.80658	-0.8231	-3.62521
H	-5.3293	-1.07123	-4.54307
C	3.22449	-2.34882	3.27486
H	2.73963	-2.59576	4.21394
C	-3.11721	2.8969	0.21094
H	-2.65217	2.89363	-0.76787
C	2.62026	-1.44434	2.4072
H	1.68613	-0.96849	2.6826
C	-0.84092	-1.24877	-12.71292
C	-0.749	-0.22329	-13.71397
C	-0.95715	-2.56387	-13.11275
C	-0.60339	1.15315	-13.39607
C	-0.78372	-0.59366	-15.0887
C	-0.97555	-2.92531	-14.47519
H	-1.06639	-3.3378	-12.36042
C	-0.52285	2.1043	-14.37974
H	-0.54155	1.46009	-12.35857
C	-0.69699	0.41421	-16.08365
C	-0.89591	-1.96212	-15.44355
H	-1.07022	-3.97129	-14.74777
C	-0.57354	1.73371	-15.74167
H	-0.72791	0.11506	-17.12727
H	-0.92159	-2.22906	-16.49581
H	-0.50834	2.49573	-16.51139
H	-0.41326	3.15019	-14.11178

Table S9: Computational result of optimized structure of complex **4**

Atoms	**Coordinates (Angstroms)**		
	X	**Y**	**Z**
Ru	-1.55185	-0.2132	-0.43112
Cl	0.87774	-0.25903	0.25638
P	-1.55768	2.25613	-0.31402
P	-1.36605	-2.67674	-0.58477
N	-1.61154	-0.02924	-2.57661
C	-3.6824	-0.43618	1.56684
C	-8.52551	-1.16916	-0.79797
H	-8.09958	-1.86787	-0.08509
C	-5.72311	-0.42939	0.03367
H	-6.4057	-0.53274	0.86715
N	-3.51239	-0.24103	-0.79114
C	-10.47448	-0.3124	-1.95716
N	-2.32475	-0.35448	1.53781
C	1.7558	-3.14519	-3.22649
H	2.66934	-2.60899	-3.46291
C	-6.22929	-0.28806	-1.26175
C	-1.34012	3.04698	1.33528
C	-4.35422	-0.38669	0.24812

C	-2.88357	0.01805	-3.05825
C	-7.68716	-0.30329	-1.50945
C	-0.59637	0.05989	-3.44144
H	0.39494	0.01405	-3.01347
C	-1.64571	-0.35972	2.68738
H	-0.56835	-0.31618	2.5898
C	-1.78205	4.76884	2.97797
H	-2.35403	5.63632	3.29105
C	-11.92131	-0.26089	-2.20919
H	-12.21622	0.26488	-3.11466
C	0.90004	-2.64612	-2.24975
H	1.16034	-1.74248	-1.71068
C	-0.28004	-3.32261	-1.92604
C	-4.36858	-0.53185	2.77026
H	-5.44854	-0.60212	2.78115
C	-2.27453	-0.43681	3.92273
H	-1.67926	-0.4332	4.82759
C	-3.13686	0.15281	-4.41742
H	-4.15492	0.18451	-4.78298
C	-3.15563	2.90938	-0.9472
C	-0.91261	-4.05409	3.27125
H	-1.48293	-4.00548	4.19313
C	-0.30777	3.19597	-1.28776
C	-5.32257	-0.1154	-2.31035
H	-5.68843	-0.01838	-3.32392
C	-8.26009	0.54785	-2.45809
H	-7.63508	1.24393	-3.00799
C	-4.77428	-3.89922	-2.50421
H	-5.2312	-3.68748	-3.46543
C	-0.03358	3.16618	3.37059
H	0.76656	2.77655	3.99177
C	-0.47974	4.56738	-1.51623
H	-1.37216	5.07214	-1.16194
C	-9.89184	-1.17861	-1.02249
H	-10.50978	-1.88404	-0.47789
C	-0.31476	2.55888	2.15202
H	0.27613	1.7117	1.81936
C	0.31256	-4.71123	3.2382
H	0.70535	-5.17901	4.13501
C	0.48409	5.29541	-2.19948
H	0.33431	6.3561	-2.37265
C	1.0289	-4.76551	2.04881
H	1.98572	-5.27585	2.01116
C	-3.96028	-0.10455	-2.04918
C	-2.95155	-3.55442	-0.93758
C	-3.57034	-3.2961	-2.16759
H	-3.09087	-2.64132	-2.88704
C	-3.65667	-0.52879	3.96401
H	-4.18106	-0.59784	4.91026
C	-9.62904	0.53975	-2.67694
H	-10.05711	1.2181	-3.40866
C	-0.77127	4.26778	3.7905

H	-0.55385	4.73956	4.74333
C	-2.06169	4.16807	1.755
H	-2.84314	4.58519	1.13144
C	-5.65065	3.69589	-1.96382
H	-6.61334	4.01125	-2.35285
C	1.64078	4.66759	-2.65575
H	2.3948	5.23798	-3.18855
C	-4.29622	2.90027	-0.13484
H	-4.22422	2.59411	0.90365
C	-0.78116	0.19986	-4.80919
H	0.08062	0.26744	-5.46174
C	0.28038	-5.01164	-3.56983
H	0.03468	-5.93893	-4.07712
C	-12.87639	-0.75685	-1.41328
H	-12.58706	-1.22082	-0.47248
C	-3.29401	3.2965	-2.28399
H	-2.43131	3.3046	-2.94055
C	-5.52998	3.2968	-0.63623
H	-6.39913	3.29318	0.01331
C	-2.07443	0.2471	-5.30564
H	-2.25919	0.3538	-6.36845
C	-0.57443	-4.51792	-2.5911
H	-1.47322	-5.07176	-2.34779
C	0.52517	-4.17019	0.8969
H	1.09797	-4.22752	-0.02035
C	-4.53055	3.68931	-2.78649
H	-4.61315	3.99577	-3.82416
C	-0.70294	-3.50455	0.91738
C	-4.77741	-5.05317	-0.39783
H	-5.23637	-5.74955	0.29642
C	-3.5668	-4.45156	-0.06262
H	-3.10176	-4.70559	0.88083
C	1.44555	-4.32465	-3.89357
H	2.11196	-4.71169	-4.65768
C	-5.38792	-4.77557	-1.61379
H	-6.32963	-5.24767	-1.87379
C	1.82974	3.31334	-2.41487
H	2.73608	2.8206	-2.75197
C	-1.41177	-3.45044	2.12346
H	-2.37151	-2.94996	2.17327
C	0.86168	2.58005	-1.73239
H	1.03276	1.53534	-1.50593
H	-14.10739	-2.71324	-5.81849
C	-14.71232	-2.22803	-5.05919
C	-14.12959	-1.78791	-3.90932
C	-16.11081	-2.07089	-5.27554
C	-14.89545	-1.15108	-2.87859
H	-13.06823	-1.93305	-3.75683
C	-16.88329	-1.49947	-4.31344
H	-16.55438	-2.42135	-6.2017
C	-14.32902	-0.67745	-1.67399
C	-16.31306	-1.03586	-3.08584

H	-17.95449	-1.38881	-4.45366
C	-15.16263	-0.13407	-0.6703
C	-17.11594	-0.48765	-2.08975
C	-14.64513	0.36801	0.5664
C	-16.5769	-0.04541	-0.88367
H	-18.18699	-0.40775	-2.25473
C	-15.46842	0.88591	1.52133
H	-13.57566	0.34784	0.73922
C	-17.40697	0.5075	0.14047
C	-16.87408	0.95506	1.30999
H	-15.05058	1.25803	2.45124
H	-18.47647	0.56295	-0.03983
H	-17.51288	1.37247	2.08133

Table S10: Computational result of optimized structure of complex **5**

Atoms	**Coordinates (Angstroms)**		
	X	**Y**	**Z**
Ru	-0.00505	0.15598	-0.04181
P	-0.07115	0.25695	2.40224
P	0.30391	0.32194	-2.46888
N	-1.5608	1.67081	-0.11207
C	-0.21242	-2.7759	-0.12266
C	-5.29964	-4.46144	-1.09608
H	-4.43738	-4.76967	-1.67874
C	-2.74687	-3.0766	-0.25595
H	-2.66926	-4.15607	-0.25014
N	-1.71811	-0.9469	-0.1707
C	-7.60025	-4.84555	-0.42972
N	0.75149	-1.81759	-0.02728
C	1.07733	4.33938	-2.92291
H	1.55943	5.11572	-2.33731
C	-4.00902	-2.4731	-0.28413
C	1.25236	-0.66717	3.29017
C	-1.6093	-2.28504	-0.19583
C	-2.81615	1.14566	-0.18086
C	-5.24131	-3.28969	-0.3324
C	-1.42769	3.0014	-0.09186
H	-0.41527	3.37356	-0.03617
C	2.03244	-2.18547	0.06872
H	2.74253	-1.37074	0.14487
C	2.38451	-2.75345	3.79997
H	2.45502	-3.82929	3.67749
C	-8.85434	-5.607	-0.44725
H	-9.61524	-5.23571	0.23496
C	0.9762	3.05168	-2.40571
H	1.3986	2.82063	-1.43422
C	0.36337	2.03517	-3.14481
C	0.12174	-4.12418	-0.13245
H	-0.6511	-4.87784	-0.21277
C	2.42643	-3.51653	0.06941

H	3.47815	-3.76271	0.15017
C	-3.93848	1.96307	-0.23445
H	-4.92726	1.52701	-0.29168
C	-1.65839	-0.36011	3.12559
C	3.24141	-2.37997	-3.50453
H	3.38442	-3.4523	-3.41984
C	0.03388	1.92859	3.17139
C	-4.07813	-1.07774	-0.25814
H	-5.04344	-0.59032	-0.30037
C	-6.37701	-2.91149	0.38798
H	-6.34976	-2.02549	1.01414
C	-3.38878	-0.39057	-4.10148
H	-4.3692	0.06504	-4.00712
C	3.20057	-0.69793	4.73426
H	3.91327	-0.15749	5.34858
C	-0.48863	2.15603	4.45093
H	-0.99609	1.3585	4.98165
C	-10.38275	-7.4319	-1.24169
C	-6.45458	-5.22289	-1.14472
H	-6.46093	-6.12319	-1.74894
C	-11.71564	-9.16768	-2.2975
H	-11.82082	-9.92522	-3.06755
C	2.18523	0.0006	4.08954
H	2.12357	1.07416	4.21636
C	-12.74432	-8.94709	-1.38871
C	4.22608	-1.58451	-4.07969
H	5.14332	-2.03189	-4.4483
C	-0.3638	3.39981	5.05652
H	-0.77591	3.55777	6.04784
C	4.02566	-0.21282	-4.18045
H	4.78556	0.41798	-4.63025
C	-2.90739	-0.3339	-0.20231
C	-1.03777	-0.43061	-3.49245
C	-2.31807	0.12881	-3.38698
H	-2.47737	1.00246	-2.76507
C	1.45666	-4.50066	-0.03573
H	1.72715	-5.55049	-0.0412
C	-7.53056	-3.67859	0.34124
H	-8.39832	-3.37144	0.91707
C	3.30071	-2.07704	4.59731
H	4.09009	-2.62162	5.1049
C	1.37818	-2.05409	3.14436
H	0.68796	-2.6061	2.51807
C	-10.54792	-8.41851	-2.2214
H	-9.74727	-8.59534	-2.93402
C	-4.17248	-1.22149	4.04118
H	-5.14159	-1.5545	4.39808
C	0.28927	4.43665	4.3965
H	0.38552	5.40843	4.86998
C	-1.81133	-1.61241	3.72419
H	-0.958	-2.26173	3.86905
C	-2.50722	3.87148	-0.13893

H	-2.33459	4.94058	-0.11891
C	-0.03558	3.62407	-4.93004
H	-0.42859	3.83905	-5.91844
C	-9.12941	-6.66698	-1.21909
H	-8.37849	-7.01735	-1.92374
C	-2.78964	0.45833	3.0061
H	-2.69861	1.45135	2.58013
C	-3.05765	-2.03904	4.17532
H	-3.14955	-3.01377	4.64346
C	-3.7862	3.34242	-0.21276
H	-4.6555	3.98888	-0.25304
C	-0.13298	2.33531	-4.41816
H	-0.59797	1.56302	-5.01938
C	2.84784	0.36184	-3.71271
H	2.71069	1.43208	-3.80562
C	-4.032	0.03475	3.45979
H	-4.89043	0.69186	3.36347
C	1.85095	-0.42591	-3.13053
C	-1.93626	-2.04189	-5.06487
H	-1.77397	-2.8848	-5.72884
C	-0.86112	-1.5165	-4.35189
H	0.119	-1.95371	-4.49045
C	-12.59249	-7.97371	-0.40334
H	-13.38813	-7.79937	0.31403
C	0.56656	4.63069	-4.18264
H	0.64255	5.63622	-4.58384
C	-3.20268	-1.48662	-4.93885
H	-4.0381	-1.89589	-5.49733
C	0.82398	4.2179	3.13294
H	1.34512	5.01697	2.61529
C	2.06899	-1.8049	-3.02824
H	1.3158	-2.44746	-2.58745
C	-11.42635	-7.2263	-0.32823
H	-11.32611	-6.48176	0.45447
C	0.69893	2.97186	2.52376
H	1.15033	2.79331	1.55573
C	1.83632	1.05926	0.1092
C	2.98511	1.47321	0.21515
C	4.31869	1.98166	0.34496
C	5.27805	1.75906	-0.65605
C	4.70107	2.71754	1.4784
C	6.56908	2.25385	-0.52539
H	4.99581	1.19254	-1.53776
C	5.9931	3.21079	1.60367
H	3.96922	2.89837	2.25926
C	6.93417	2.98169	0.60373
H	7.29576	2.0699	-1.31095
H	6.26769	3.77736	2.48828
H	7.94373	3.36717	0.70366
H	-13.6575	-9.53068	-1.4433

Table S11: Computational result of optimized structure of complex **6**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.0005	0.16763	-0.03833
P	-0.0608	0.26432	2.40598
P	0.30726	0.3332	-2.46593
N	-1.53191	1.70758	-0.10513
C	-0.25567	-2.76048	-0.12138
C	-5.36676	-4.36491	-1.10334
H	-4.50425	-4.69453	-1.67379
C	-2.79493	-3.0198	-0.25834
H	-2.73507	-4.10045	-0.25325
N	-1.73115	-0.90727	-0.16822
C	-7.68445	-4.69626	-0.46659
N	0.72387	-1.81794	-0.02715
C	1.14259	4.33905	-2.91253
H	1.63485	5.10728	-2.32469
C	-4.047	-2.39558	-0.2905
C	1.25497	-0.67557	3.28881
C	-1.64457	-2.24702	-0.19475
C	-2.79538	1.20293	-0.17701
C	-5.29347	-3.18942	-0.34657
C	-1.3774	3.03576	-0.08008
H	-0.35917	3.39126	-0.02117
C	1.99886	-2.20669	0.06614
H	2.72224	-1.40372	0.14162
C	2.36433	-2.7754	3.7929
H	2.4218	-3.85189	3.66929
C	-8.95523	-5.42846	-0.49739
H	-9.72942	-5.01034	0.14137
C	1.02061	3.05237	-2.39723
H	1.43706	2.81348	-1.42512
C	0.39426	2.04628	-3.1391
C	0.05666	-4.11395	-0.13203
H	-0.72857	-4.85475	-0.21132
C	2.3713	-3.54395	0.06523
H	3.41908	-3.80717	0.1436
C	-3.9045	2.03839	-0.22929
H	-4.90012	1.61838	-0.28876
C	-1.65195	-0.33741	3.13329
C	3.19841	-2.41488	-3.5114
H	3.32473	-3.48934	-3.42729
C	0.06527	1.93347	3.17761
C	-4.09249	-0.99921	-0.263
H	-5.04918	-0.49563	-0.30858
C	-6.43099	-2.78285	0.35537
H	-6.39422	-1.89299	0.97556
C	-3.39914	-0.30722	-4.09694
H	-4.36989	0.16892	-4.00392
C	3.20743	-0.73037	4.72633
H	3.9284	-0.19893	5.33884

C	-0.45849	2.16741	4.45538
H	-0.97979	1.37712	4.98345
C	-10.49913	-7.25006	-1.27187
C	-6.53698	-5.10175	-1.16357
H	-6.55489	-6.00301	-1.76614
C	-11.81088	-9.04908	-2.24563
H	-11.87951	-9.87728	-2.94509
C	2.19804	-0.01944	4.08585
H	2.14904	1.05462	4.21408
C	-12.90834	-8.73203	-1.4479
C	4.19374	-1.63494	-4.08943
H	5.10269	-2.09661	-4.46092
C	-0.31723	3.40858	5.06285
H	-0.73071	3.57166	6.05277
C	4.01467	-0.26022	-4.18924
H	4.78306	0.35862	-4.64125
C	-2.91015	-0.27486	-0.202
C	-1.0494	-0.39407	-3.48805
C	-2.31784	0.19193	-3.38396
H	-2.45881	1.07043	-2.76442
C	1.38544	-4.51218	-0.038
H	1.63874	-5.56627	-0.0443
C	-7.6	-3.5251	0.29689
H	-8.46912	-3.19486	0.85771
C	3.29119	-2.11041	4.58751
H	4.07602	-2.6646	5.09176
C	1.36388	-2.06371	3.14156
H	0.66442	-2.60689	2.51781
C	-10.62938	-8.32279	-2.15928
H	-9.78892	-8.59165	-2.79316
C	-4.17086	-1.17314	4.05892
H	-5.14192	-1.49628	4.41954
C	0.354	4.43609	4.40658
H	0.46314	5.4058	4.88152
C	-1.8135	-1.58465	3.74006
H	-0.96491	-2.23959	3.88738
C	-2.44275	3.9232	-0.12575
H	-2.25295	4.98931	-0.10186
C	0.02435	3.6431	-4.92354
H	-0.36267	3.86519	-5.91273
C	-9.22911	-6.51662	-1.23011
H	-8.45815	-6.92221	-1.88171
C	-14.19917	-9.50013	-1.54596
H	-14.57477	-9.77391	-0.55598
H	-14.07458	-10.41563	-2.1281
H	-14.97742	-8.90122	-2.03067
C	-2.77686	0.48928	3.01085
H	-2.6786	1.47896	2.57877
C	-3.06235	-1.99866	4.19605
H	-3.16107	-2.96974	4.67034
C	-3.72998	3.41504	-0.20311
H	-4.58868	4.07559	-0.24246

C	-0.09402	2.35542	-4.41347
H	-0.56913	1.59095	-5.01681
C	2.84753	0.33282	-3.71774
H	2.72707	1.40511	-3.81007
C	-4.0216	0.0784	3.46955
H	-4.87504	0.74164	3.37091
C	1.84008	-0.4392	-3.13258
C	-1.98127	-1.99132	-5.05527
H	-1.8366	-2.83949	-5.71661
C	-0.8954	-1.48624	-4.34387
H	0.07546	-1.94406	-4.48111
C	-12.77832	-7.66291	-0.55425
H	-13.61655	-7.39961	0.08511
C	0.63967	4.63958	-4.17323
H	0.732	5.64432	-4.57298
C	-3.23585	-1.40934	-4.93108
H	-4.07959	-1.80278	-5.48841
C	0.89036	4.21055	3.14488
H	1.4257	5.00215	2.63025
C	2.03672	-1.82147	-3.03127
H	1.27511	-2.45218	-2.58793
C	-11.60293	-0.46489	-6.93652
H	-11.54389	-6.11958	0.24674
C	0.74876	2.96727	2.53376
H	1.2012	2.78311	1.5672
C	1.85486	1.0424	0.11141
C	3.00993	1.43903	0.21559
C	4.35137	1.92684	0.34343
C	5.30241	1.7001	-0.66458
C	4.75005	2.64606	1.48194
C	6.60109	2.17495	-0.53581
H	5.00767	1.14606	-1.55011
C	6.04967	3.11944	1.60529
H	4.02485	2.82962	2.26835
C	6.98228	2.88657	0.59832
H	7.32112	1.98813	-1.32679
H	6.33689	3.67335	2.49392
H	7.9978	3.2565	0.69673

Table S12: Computational result of optimized structure of complex **7**

Atoms	**Coordinates (Angstroms)**		
	X	**Y**	**Z**
Ru	-0.02573	0.17243	-0.12117
P	-0.14745	0.11332	2.32396
P	0.34827	0.48621	- 2.52093
N	-1.54681	1.72332	-0.11911
C	-0.29448	-2.7429	-0.40052
C	-5.40738	-4.25403	-1.51214
H	-4.55297	-4.5345	-2.1198
C	-2.83298	-2.97809	-0.57897
H	-2.77923	-4.05745	-0.6398

N	-1.75902	-0.88127	-0.34989
C	-7.71143	-4.64182	-0.86256
N	0.68745	-1.81545	-0.22142
C	1.1816	4.51313	-2.69865
H	1.66928	5.24125	-2.05828
C	-4.08137	-2.3463	-0.57606
C	1.12794	-0.91225	3.17026
C	-1.67918	-2.21708	-0.46004
C	-2.81199	1.232	-0.23931
C	-5.32985	-3.13329	-0.67744
C	-1.38542	3.04655	-0.01288
H	-0.36611	3.39132	0.08179
C	1.95785	-2.21842	-0.12626
H	2.68415	-1.42753	0.01778
C	2.18392	-3.06393	3.55715
H	2.22213	-4.13102	3.36403
C	-8.96767	-5.39985	-0.91009
H	-9.82337	-4.90374	-0.45706
C	1.05857	3.19512	-2.27058
H	1.46851	2.89331	-1.31314
C	0.43829	2.23948	-3.08159
C	0.01086	-4.09443	-0.49872
H	-0.77645	-4.82235	-0.6467
C	2.32305	-3.55513	-0.20947
H	3.36734	-3.83022	-0.12523
C	-3.91542	2.07637	-0.26116
H	-4.9123	1.6673	-0.36264
C	-1.76984	-0.49705	2.9717
C	3.28235	-2.17408	-3.6607
H	3.40715	-3.25197	-3.65456
C	-0.00872	1.72272	3.21065
C	-4.1203	-0.95417	-0.46319
H	-5.07397	-0.44324	-0.47814
C	-6.4627	-2.7728	0.05698
H	-6.42268	-1.92331	0.73121
C	-3.30584	-0.11678	-4.27705
H	-4.29425	0.31454	-4.15567
C	3.04982	-1.10263	4.63743
H	3.7692	-0.62765	5.29645
C	-0.53435	1.8689	4.50088
H	-1.06083	1.04585	4.97076
C	-6.57687	-4.98913	-1.60856
H	-6.61256	-5.83193	-2.29015
C	2.06844	-0.32989	4.02574
H	2.03949	0.73443	4.22273
C	4.29802	-1.35341	-4.13844
H	5.2214	-1.78655	-4.50872
C	-0.38813	3.06344	5.19415
H	-0.80259	3.15881	6.19244
C	4.12048	0.02516	-4.14064
H	4.90455	0.67559	-4.51465
C	-2.93444	-0.24123	-0.35299

C	-0.96534	-0.18851	-3.63138
C	-2.25483	0.34148	-3.49464
H	-2.43623	1.14631	-2.79158
C	1.33505	-4.50721	-0.40293
H	1.58305	-5.55998	-0.47682
C	-7.63019	-3.51409	-0.03697
H	-8.49531	-3.22414	0.5516
C	3.10753	-2.47239	4.41132
H	3.8701	-3.07514	4.89351
C	1.21236	-2.28979	2.93384
H	0.51806	-2.77574	2.25909
C	-4.32984	-1.33098	3.7787
H	-5.31683	-1.6537	4.09355
C	0.28913	4.1313	4.61225
H	0.40184	5.06478	5.1542
C	-1.97813	-1.78336	3.47364
H	-1.15077	-2.47182	3.58468
C	-2.44506	3.94201	-0.02224
H	-2.24971	5.00358	0.06761
C	0.07561	3.95107	-4.7577
H	-0.30658	4.23789	-5.73202
C	-9.13133	-6.6302	-1.41452
H	-8.26616	-7.16044	-1.80338
C	-2.86892	0.36897	2.89441
H	2.73526	1.38683	2.54503
C	-3.24715	-2.19628	3.87101
H	-3.38235	-3.19871	4.26408
C	-3.73362	3.44786	-0.15063
H	-4.58776	4.11528	-0.16519
C	-0.04346	2.63194	-4.33502
H	-0.51322	1.90837	-4.99057
C	2.93496	0.58211	-3.67089
H	2.81587	1.65843	-3.6864
C	-4.13397	-0.04138	3.29454
H	-4.96674	0.65197	3.23307
C	1.90764	-0.23119	-3.18533
C	-1.8133	-1.64506	-5.37354
H	-1.62771	-2.4154	-6.11505
C	-0.75809	-1.18037	-4.59189
H	0.23013	-1.59054	-4.75404
C	0.68526	4.89615	-3.93962
H	0.77822	5.92533	-4.27121
C	-3.08952	-1.12109	-5.21609
H	-3.90927	-1.48306	-5.82789
C	0.82642	3.99248	3.3386
H	1.36602	4.81575	2.88134
C	2.10195	-1.61739	-3.18239
H	1.32272	-2.27812	-2.8205
C	0.68049	2.79544	2.64193
H	1.13422	2.676	1.66613
C	-10.42162	-7.33431	-1.48402
C	-10.49002	-8.75798	-1.31107

C	-11.58293	-6.63591	-1.7408
C	-9.35068	-9.55286	-1.01697
C	-11.75296	-9.40772	-1.41542
C	-12.83268	-7.28286	-1.82728
H	-11.5298	-5.5655	-1.90931
C	-9.45386	-10.91078	-0.86144
H	-8.38332	-9.07879	-0.89902
C	-11.82716	-10.81489	-1.2492
C	-12.91697	-8.63971	-1.674
H	-13.72273	-6.69723	-2.0328
C	-10.70588	-11.55322	-0.9824
H	-12.79704	-11.2961	-1.33529
H	-13.87305	-9.14874	-1.75093
H	-10.77495	-12.62883	-0.85697
H	-8.56876	-11.49765	-0.63795
C	1.82924	1.02579	0.13036
C	2.98184	1.40991	0.2923
C	4.31977	1.8839	0.49078
C	5.30808	1.69135	-0.48807
C	4.67737	2.55545	1.67132
C	6.60282	2.15343	-0.291
H	5.04544	1.17464	-1.40567
C	5.97324	3.01629	1.86288
H	3.92336	2.71205	2.43618
C	6.943	2.81796	0.88397
H	7.35197	1.9938	-1.06061
H	6.22827	3.53327	2.78301
H	7.95542	3.17819	1.03572

Table S13: Computational result of optimized structure of complex **8**

Atoms	**Coordinates (Angstroms)**		
	X	**Y**	**Z**
Ru	-1.64146	0.19396	-0.37032
P	-1.81859	0.1011	2.0655
P	-1.22995	0.41586	-2.77647
N	-2.47089	2.19799	-0.26642
C	-2.998	-2.39864	-0.72874
C	-8.24452	-1.76942	-2.04686
H	-7.53108	-2.29654	-2.67211
C	-5.42587	-1.63969	-0.97733
H	-5.78135	-2.65126	-1.1244
N	-3.64801	-0.12477	-0.5986
C	-10.55112	-1.31981	-1.45195
N	-1.73982	-1.92132	-0.51907
C	0.9199	3.92134	-2.9423
H	1.65189	4.42102	-2.31573
C	-6.34284	-0.58525	-0.93114
C	-1.1422	-1.38083	2.92858
C	-4.07541	-1.38197	-0.79055
C	-3.8304	2.21953	-0.3469
C	-7.79003	-0.83402	-1.1102

C	-1.82415	3.35732	-0.10657
H	-0.74728	3.29286	-0.05292
C	-0.72581	-2.78532	-0.41471
H	0.24997	-2.34023	-0.26919
C	-1.18103	-3.09259	4.63977
H	-1.70235	-3.58983	5.45144
C	-11.99782	-1.54351	-1.58013
H	-12.624	-0.81857	-1.06468
C	0.37136	2.71241	-2.5267
H	0.69174	2.26309	-1.59333
C	-0.56968	2.04836	-3.32041
C	-3.23496	-3.7626	-0.84419
H	-4.2384	-4.13066	-1.01454
C	-0.90164	-4.15889	-0.50648
H	-0.04557	-4.81569	-0.41134
C	-4.5393	3.41183	-0.26487
H	-5.61952	3.40851	-0.33013
C	-3.58241	0.18504	2.57924
C	0.62559	-3.0584	-3.98457
H	0.38785	-4.11713	-3.97342
C	-1.024	1.43025	3.06543
C	-5.86029	0.70593	-0.7018
H	-6.55162	1.53795	-0.67649
C	-8.73578	-0.13891	-0.35241
H	-8.40943	0.57522	0.39701
C	-4.91433	1.08551	-4.44132
H	-5.70264	1.81576	-4.28979
C	0.7574	-2.85117	3.23885
H	1.75787	-3.1587	2.95161
C	-1.36136	1.59305	4.41507
H	-2.12813	0.97076	4.86431
C	-9.59822	-2.00288	-2.21943
H	-9.91586	-2.71263	-2.9754
C	0.14543	-1.7961	2.57219
H	0.67428	-1.27586	1.78016
C	1.83912	-2.61785	-4.50124
H	2.55559	-3.3307	-4.89602
C	-0.72336	2.54944	5.19308
H	-0.99976	2.66586	6.23595
C	2.12543	-1.25787	-4.51163
H	3.06697	-0.90174	-4.91716
C	-4.49622	0.90984	-0.54629
C	-2.71541	0.23522	-3.85846
C	-3.7543	1.1583	-3.68267
H	-3.64507	1.96451	-2.96587
C	-2.1762	-4.655	-0.72964
H	-2.35168	-5.72154	-0.81313
C	-10.09068	-0.37949	-0.52303
H	-10.80977	0.16263	0.08352
C	0.09294	-3.50764	4.26946
H	0.56918	-4.33367	4.78775
C	-1.79352	-2.03195	3.97968

H	-2.77989	-1.71559	4.29664
C	-6.33499	0.33698	3.11057
H	-7.39718	0.39288	3.32564
C	0.27127	3.35118	4.63857
H	0.77086	4.0975	5.24783
C	-4.39714	-0.94978	2.4778
H	-3.9676	-1.90511	2.19428
C	-2.47264	4.58017	-0.01597
H	-1.89254	5.48561	0.1139
C	-0.39265	3.82935	-4.95382
H	-0.69263	4.2572	-5.90493
C	-12.58703	-2.55436	-2.23035
H	-11.96337	-3.31686	-2.69244
C	-4.17777	1.40069	2.92956
H	-3.57643	2.29946	3.00656
C	-5.75778	-0.87656	2.74829
H	-6.36856	-1.77031	2.67369
C	-3.85605	4.60765	-0.09545
H	-4.39973	5.54312	-0.02842
C	-0.93791	2.61766	-4.54409
H	-1.65233	2.1176	-5.18705
C	1.20622	-0.34182	-4.00913
H	1.44854	0.71354	-4.03004
C	-5.54187	1.47478	3.19532
H	-5.98135	2.42721	3.4736
C	-0.0148	-0.77178	-3.4834
C	-4.03492	-0.83228	-5.58859
H	-4.13108	-1.60895	-6.3404
C	-2.86835	-0.75419	-4.83147
H	-2.07471	-1.46526	-5.02092
C	0.53514	4.48634	-4.15306
H	0.96083	5.43144	-4.47462
C	-5.0624	0.0813	-5.39377
H	-5.96906	0.02006	-5.9867
C	0.62812	3.18246	3.30706
H	1.41361	3.79166	2.87121
C	-0.28943	-2.14433	-3.47547
H	-1.23192	-2.51134	-3.08642
C	-0.01443	2.22586	2.52386
H	0.29879	2.06392	1.50037
H	-14.93482	1.40879	-4.11262
C	-15.31557	0.45796	-3.75359
C	-14.44881	-0.4885	-3.29702
C	-16.71786	0.21287	-3.77836
C	-14.91049	-1.76026	-2.82359
H	-13.38547	-0.2886	-3.30419
C	-17.20034	-0.99057	-3.36877
H	-17.3922	0.98306	-4.1381
C	-14.04558	-2.76632	-2.3372
C	-16.32295	-2.01668	-2.89502
H	-18.2651	-1.2022	-3.39884
C	-14.56977	-4.02567	-1.96663

C	-16.82085	-3.25997	-2.5161
C	-13.74434	-5.07998	-1.46013
C	-15.97765	-4.27355	-2.06622
H	-17.88982	-3.44521	-2.57735
C	-14.27103	-6.28837	-1.11319
H	-12.68167	-4.90724	-1.33782
C	-16.49246	-5.55284	-1.68956
C	-15.66768	-6.53412	-1.23256
H	-13.6228	-7.07175	-0.73388
H	-17.56176	-5.72159	-1.7763
H	-16.06843	-7.50207	-0.9501
C	0.39955	0.33911	-0.18
C	1.62027	0.32641	-0.06749
C	3.044	0.33335	0.09975
C	3.89961	-0.07372	-0.93639
C	3.61973	0.74874	1.31187
C	5.27775	-0.06411	-0.7643
H	3.46823	-0.39874	-1.8776
C	4.99833	0.75625	1.47845
H	2.96979	1.06656	2.12102
C	5.83476	0.35033	0.44226
H	5.92188	-0.38286	-1.57823
H	5.42269	1.0808	2.42369
H	6.91195	0.35662	0.57424

6. References

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