Electronic Supplementary Information (ESI) for:

Stable Ruthenium Olefin Metathesis Catalysts Bearing Symmetrical NHC Ligands with Primary and Secondary *N*-Alkyl Groups

Chiara Ambrosio,[†] Veronica Paradiso,[†] Chiara Costabile,[†] Valerio Bertolasi,[‡] Tonino Caruso,[†] and Fabia Grisi*[†]

[†]Dipartimento di Chimica e Biologia "Adolfo Zambelli", Università di Salerno, Via Giovanni Paolo II 132, I-84084 Fisciano, Salerno, Italy

[‡]Dipartimento di Chimica and Centro di Strutturistica Diffrattometrica, Università di Ferrara, Via L. Borsari 46, I-44100 Ferrara, Italy

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Experimental Procedure

General Information

All reactions involving the manipulation of organometallic compounds were carried on under inert atmosphere using standard glove box or Schlenk techniques. Toluene, methylene chloride and diethyl ether were stored on sodium benzophenone, calcium hydride and lithium aluminium hydride respectively and distilled before use. Deuterated solvents were dried using 4 Å activated molecular sieves. Ethyl oleate was purchased by Sigma Aldrich Company and filtered on neutral alumina. All other reagents and solvents were purchased by Sigma Aldrich Company or by TCI Chemicals and used without any other purification.

Purification using chromatographic column of organic molecules and organometallic compounds was carried on using silica gel 60 (230-400 mesh) purchased by Sigma Aldrich Company and silica gel 60 (230-400 mesh) purchased by TSI Cambridge. Thin layer chromatography (TLC) was accomplished using silica gel 60 aluminium foils with F254 fluorescence indicator.

NMR analysis was carried on using Bruker AVANCE 250 (250 MHz for ^{1}H; 62.5 MHz for ^{13}C), Bruker AM 300 (300 MHz for ^{1}H; 75 MHz for ^{13}C), Bruker AVANCE 400 (400 MHz for ^{1}H; 100 MHz for ^{13}C; 161.97 MHz for ^{31}P) and Bruker ASCEND 600 (600 MHz for ^{1}H; 150 MHz for ^{13}C). NMR samples were prepared dissolving about 10 mg of substance in 0.5 mL of deuterated solvent. Chemical shifts of spectra were reported as follows: chemical shift (ppm), multiplicity and integration. Multiplicity was abbreviated as follows: singlet (s), doublet (d), triplet (t), multiplet (m), broad (br), overlapped (o). ^{1}H and ^{13}C NMR chemical shifts were assigned using tetramethylsilane (TMS) as internal standard.

ESI-MS analysis was accomplished on a Waters spectrometer with an electrospray source. ESI-FT-ICR analysis of organometallic compounds was carried on Bruker Solaris XR spectrometer.

Optical rotatory power of enantiomerically pure compounds was evaluated on a JASCO P2000 polarimeter. Cyclic voltammetry analysis was carried out on a AUTOLAB PG STAT 302N potentiostat with a three electrode configuration: a platinum electrode (2 mm diameter) as working electrode, a platinum disc (2 mm diameter) as auxiliary electrode and a *quasi-reference* (PtQRE)1, calibrated with octamethyl ferrocene as internal standard. All voltammograms were recorded with a 100mV/s scan rate in dry methylene chloride using NBu_4PF_6 (0.1 M) as supporting electrolyte.

Enantiomeric excesses were evaluated using chiral gas chromatography (Agilent Technologies 6850, column Supelco β-DEX 120L*30m*0.25mm. Method for **28**: isotherm at 60°C for 60 minutes, then 5°C/min until 100°C, then isotherm at 100°C for 10 minutes. Method for **30**: isotherm

at 40°C for 100 minutes, then 1°C/min until 50°C, then isotherm at 50°C for 120 minutes, then 1°C/min until 100°C, then isotherm at 100°C for ten minutes.

Conversions and selectivities of ethenolysis reactions were determined using gas chromatography (Agilent Technologies 7890A. Column: HP 5MS UI 60m*0.25mm. Method: isotherm at 60°C for 2 minutes, then 5°C/min until 250°C, then isotherm at 250°C for 18 minutes.).

Catalysis

Ring Closing Metathesis

An NMR tube with a screw-cap septum top was charged with 0.80 mL of a solution of the catalyst (1−5mol%) in benzene-d_6. After equilibration of the sample at 60 °C in the NMR probe, 0.080 mmol of substrate (0.1 M) was injected into the tube. Conversion of each substrate was monitored over time by ^{1}H NMR.

RCM of Diethyl Diallylmalonate (**8**). A 19.3 μL portion of **8** was injected into a heated NMR tube containing 0.80 mL of catalyst solution (1 mol %). The conversion to **9** was determined by integrating the methylene protons of the reagent at δ 2.84 (dt) and of the product at δ 3.14 (s).

RCM of Diethyl Allylmethallylmalonate (**10**). A 20.5 μL portion of 10 was injected into a heated NMR tube containing 0.80 mL of catalyst solution (1 mol %). The conversion to **11** was determined by integrating the methylene protons of the reagent at δ 2.96 (d), 2.93 (s) and of the product at δ 3.18 (m), 3.07 (s).

RCM of Diethyl Dimethallylmalonate (**12**). A 21.6 μL portion of **12** was injected into a heated NMR tube containing 0.80 mL of catalyst solution (5 mol %). The conversion to **13** was determined by integrating the methylene protons of the reagent at δ 2.98 (s) and of the product at δ 3.15 (s).

RCM of (±) linalool (**14**). A 14.3 μL portion of **14** was injected into a heated NMR tube containing 0.80 mL of catalyst solution (1 mol %). The conversion to **15** was determined by integrating the methylene protons of the reagent at δ 1.13 (br s) and of the product at δ 1.26 (br s).

Cross Metathesis

Under nitrogen atmosphere, substrates were simultaneously added to a methylene chloride solution of the catalyst (2.5 mol %). The reaction mixture was refluxed under nitrogen overnight and then purified by column chromatography on silica gel (hexaneethyl acetate 9/1). *E/Z* ratios of products were determined by ^{1}H NMR.

CM of allylbenzene (**16**) and 1,4-diacetoxy-2-butene (**17**). 66 μL of **16** (1 eq.) and 160 μL of **17** (2 eq.) were added to a solution of the catalyst . *E/Z* ratio of **18** was determined integrating the signals at δ =4.55 (d) and δ =4.73 (d) (*chemical shifts* in $CDCl_3$).

CM of eugenol acetate (**19**) and 1,4-dichloro-2-butene (**20**). 47 μL of **19** (1 eq.) and 77 μL of **20** (3 eq.) were added to a solution of the catalyst . *E/Z* ratio of **21** was determined integrating the signals at δ =4.19 (d) and δ =4.06 (d) (*chemical shifts* in $CDCl_3$).

Ethenolysis of ethyl oleate (**22**).

Under nitrogen atmosphere, in an autoclave, ethyl oleate (5.4 mmol) and dodecane (150 μL) were introduced. At this point, a t = 0 sample was prepared. The autoclave was purged with ethylene three times, and then a toluene solution of the catalyst was added. The autoclave was purged with ethylene three times and then charged with a pressure of 150 psi. The reaction mixture was stirred at 50 °C for 3 h and then cooled in an ice bath and quenched with ethyl vinyl ether.

After that, GC samples were prepared in hexane. Samples were stored at −20 °C until GC analysis. Conversions, selectivities and yields were calculated using the following equations:

$$Conversion\ (\%) = 100 * (1 - \frac{Area\ (22)sample * Area\ (dodecane)t0}{Area\ (22)t0 * Area\ (dodecane)sample})$$

$$Selectivity\ (\%) = 100 * (\frac{n(23) + n(24)}{n(23) + n(24) + 2(n(25) + n(26))})$$

$$Yield\ (\%) = \frac{Conversion * Selectivity}{100}$$

$$TON = Yield\ (\%)\frac{mol\ (22)}{mol\ (cat) * 100}$$

Ring Opening Metathesis Polymerization of COD **(27)**

An NMR tube with a screw-cap septum top was charged with 0.8 mL of a benzene-d_6 solution of the catalyst (0.8 μmol) and then was equilibrated at 60°C in the NMR probe.

After that, 49.1 μL (0.40 mmol) of **27** was injected and the reaction was monitored as a function of time, determining the conversion by integrating protons in the monomer, δ= 2.22 (s), and those in the polymer, δ= 2.14 (s) and 2.11 (s). When the conversion was complete, the polymerization was quenched with a solution of ethyl vinyl ether in methanol.

Asymmetric Ring Closing Metathesis

ARCM of **28** and **30** with chloride catalyst were carried out by adding the complex (0.0028 mmol, 0.025 equiv.) to a 2.0 mL solution of the prochiral triene (1 equiv., 0.055 M) in dry CD_2Cl_2.

The flask was stirred a 40°C for two hours for **28** and for three hours for **30**. Yields were determined via ^{1}H NMR spectroscopy of the crude product. The reaction mixture was filtered on neutral alumina and injected into the GC system without further purifications.

ARCM of **28** with iodide catalyst were carried out by adding NaI (0.055 mmol, 1 equiv.) to a 1.0 mL THF-d_8 solution of the chloride complex (0.0022 mmol, 0.04 equiv.). The reaction mixture was stirred at room temperature for one hour. After that, **28** (0.055 mmol, 1 equiv.) was added. Then, the flask was stirred a 40 °C for two hours. Yields were determined by ^{1}H NMR spectroscopy of the crude product. The reaction mixture was filtered on neutral alumina and injected into the GC system without further purifications.

NMR spectra

Figure S1: ^{1}H NMR of **A** (CD_2Cl_2, 300 MHz).

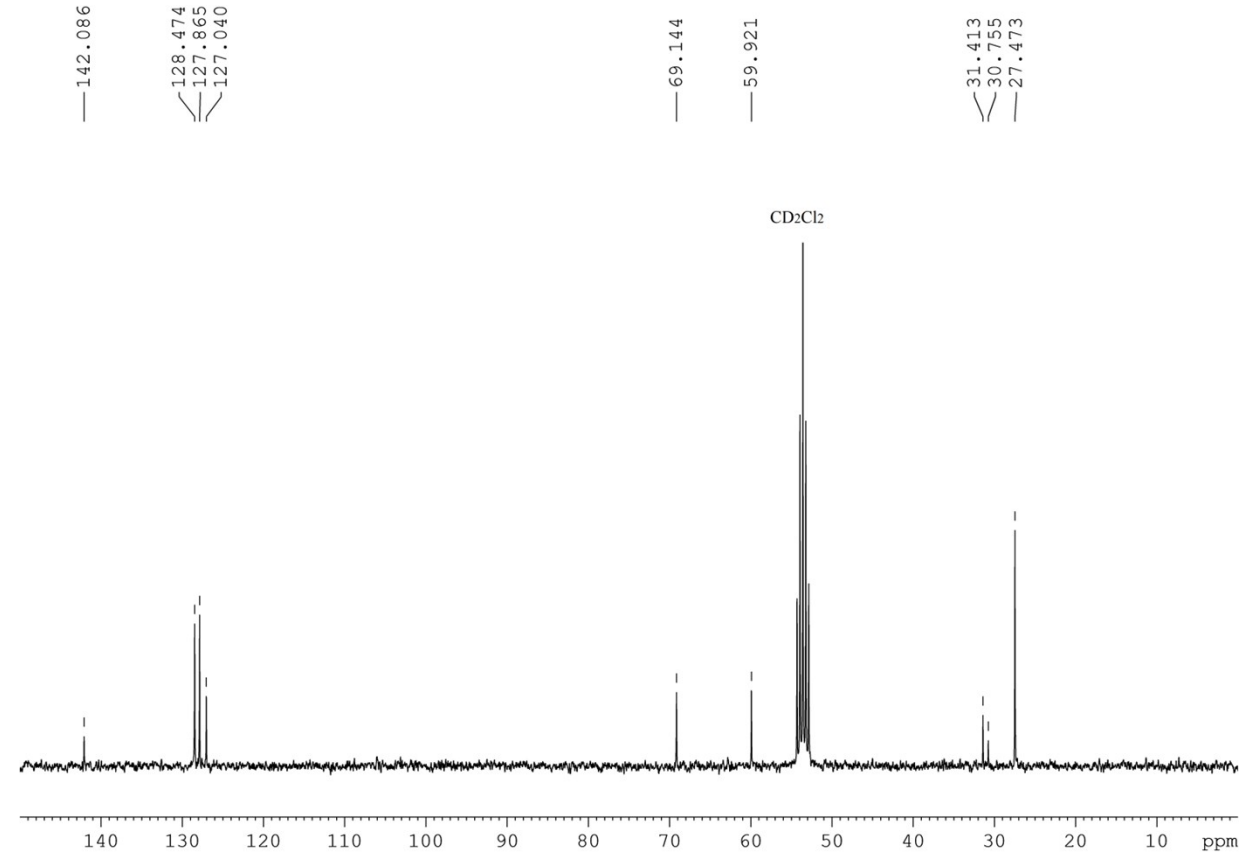

Figure S2: ^{13}C{H}NMR of **A** (CD_2Cl_2, 75 MHz).

Figure S3: ^{1}H NMR of **B** ($CDCl_3$, 300 MHz).

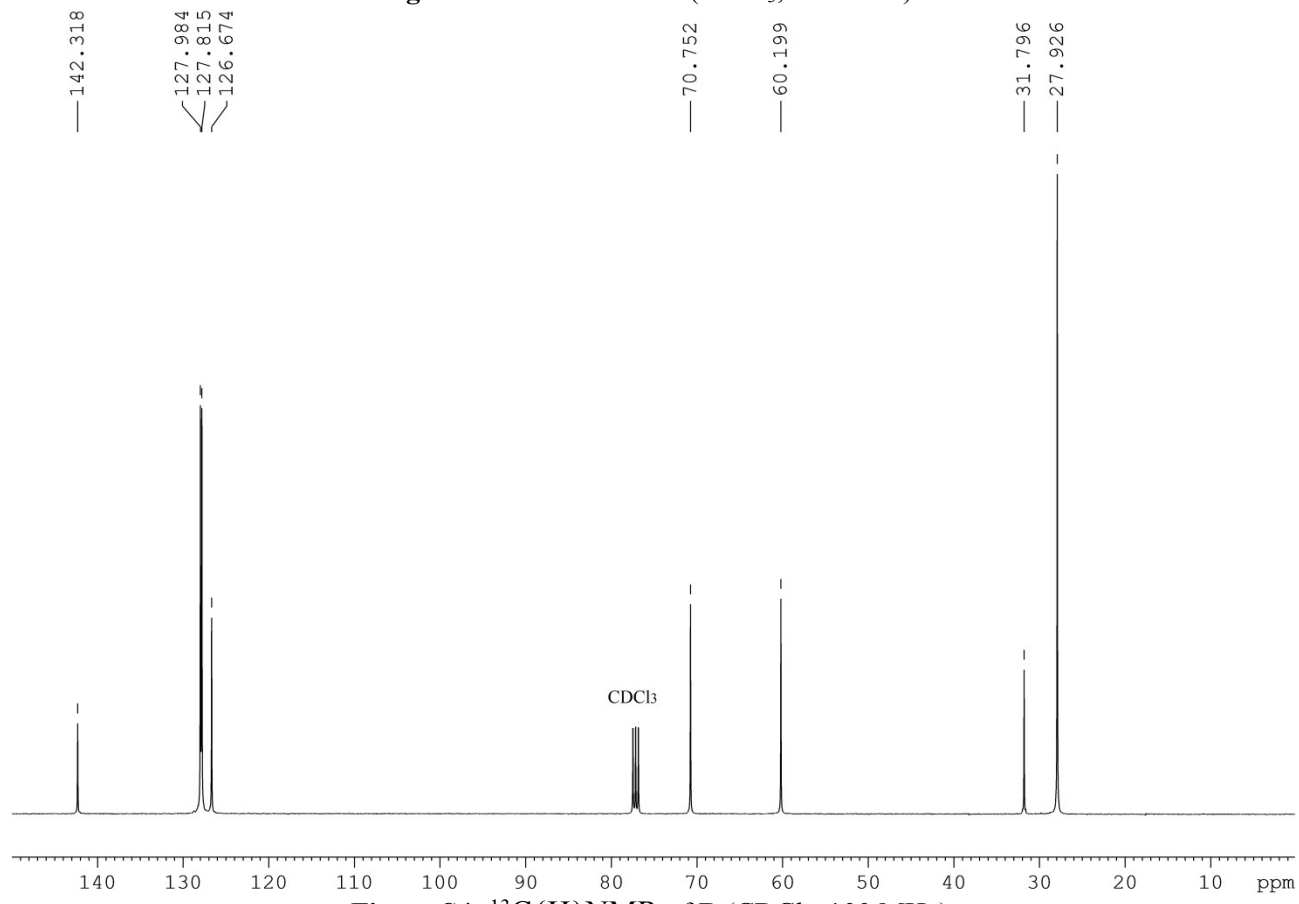

Figure S4: ^{13}C{H}NMR of **B** ($CDCl_3$, 100 MHz).

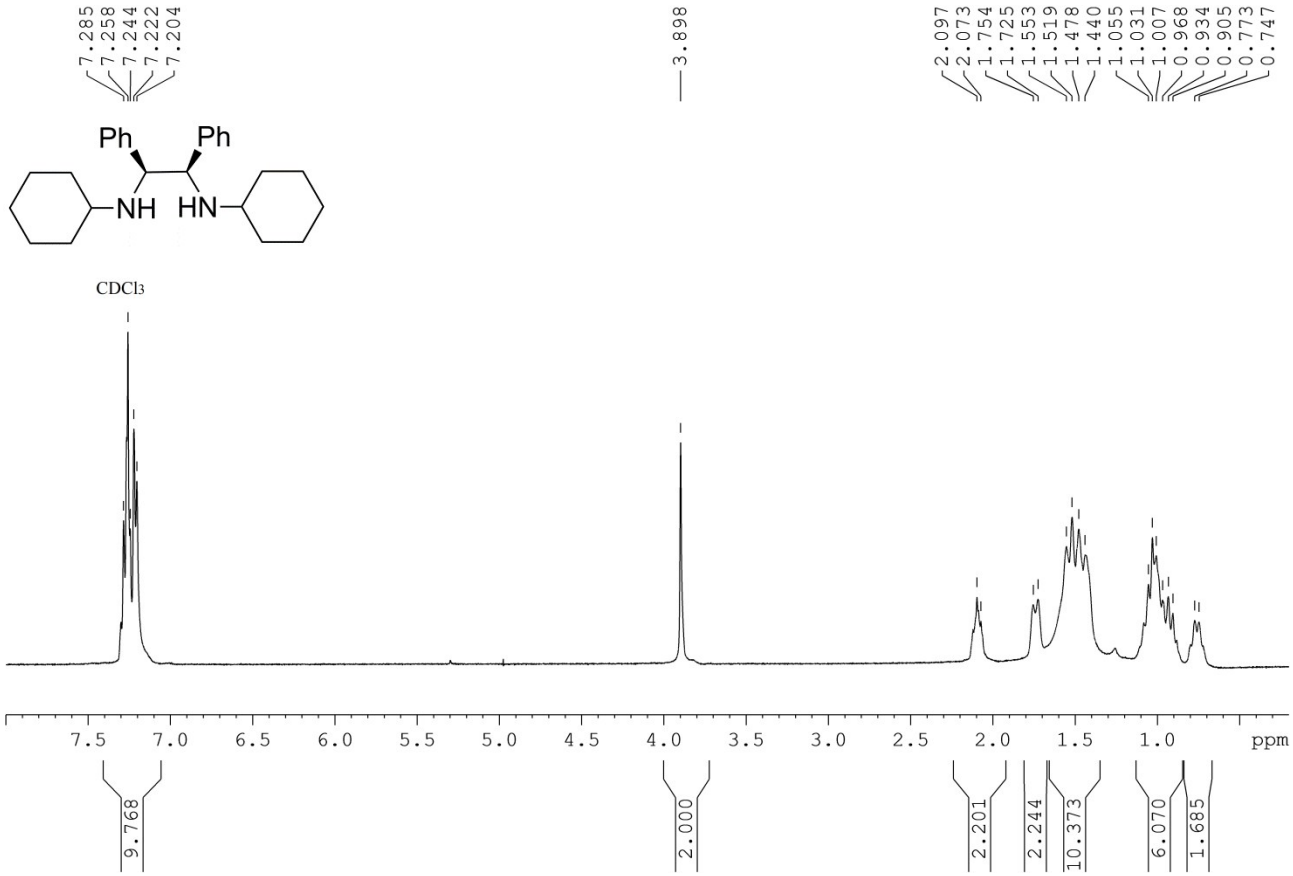

Figure S5: ^{1}H NMR of **C** ($CDCl_3$, 400 MHz).

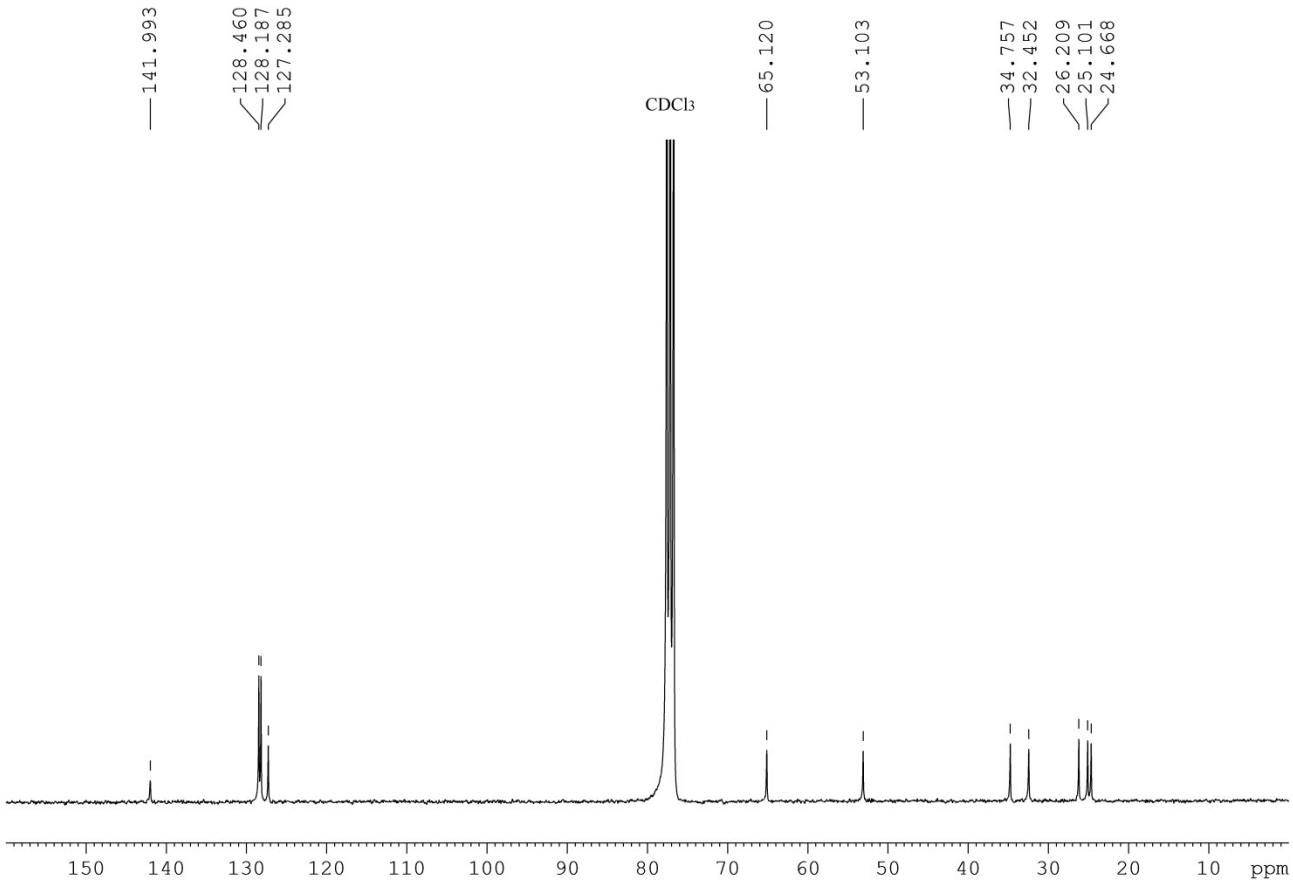

Figure S6: ^{13}C{H}NMR of **C** ($CDCl_3$, 75 MHz).

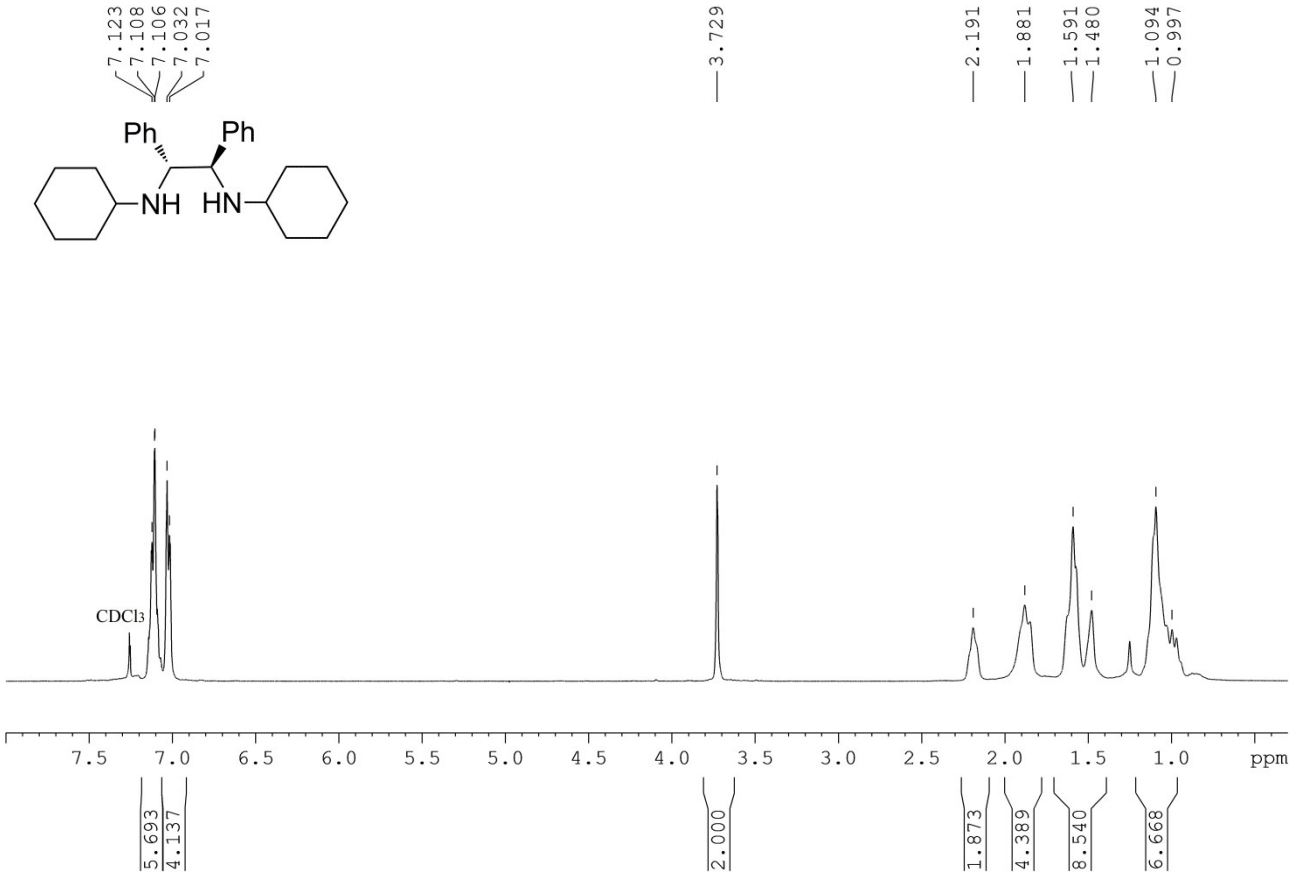

Figure S7: ^{1}H NMR of **D** ($CDCl_3$, 400 MHz).

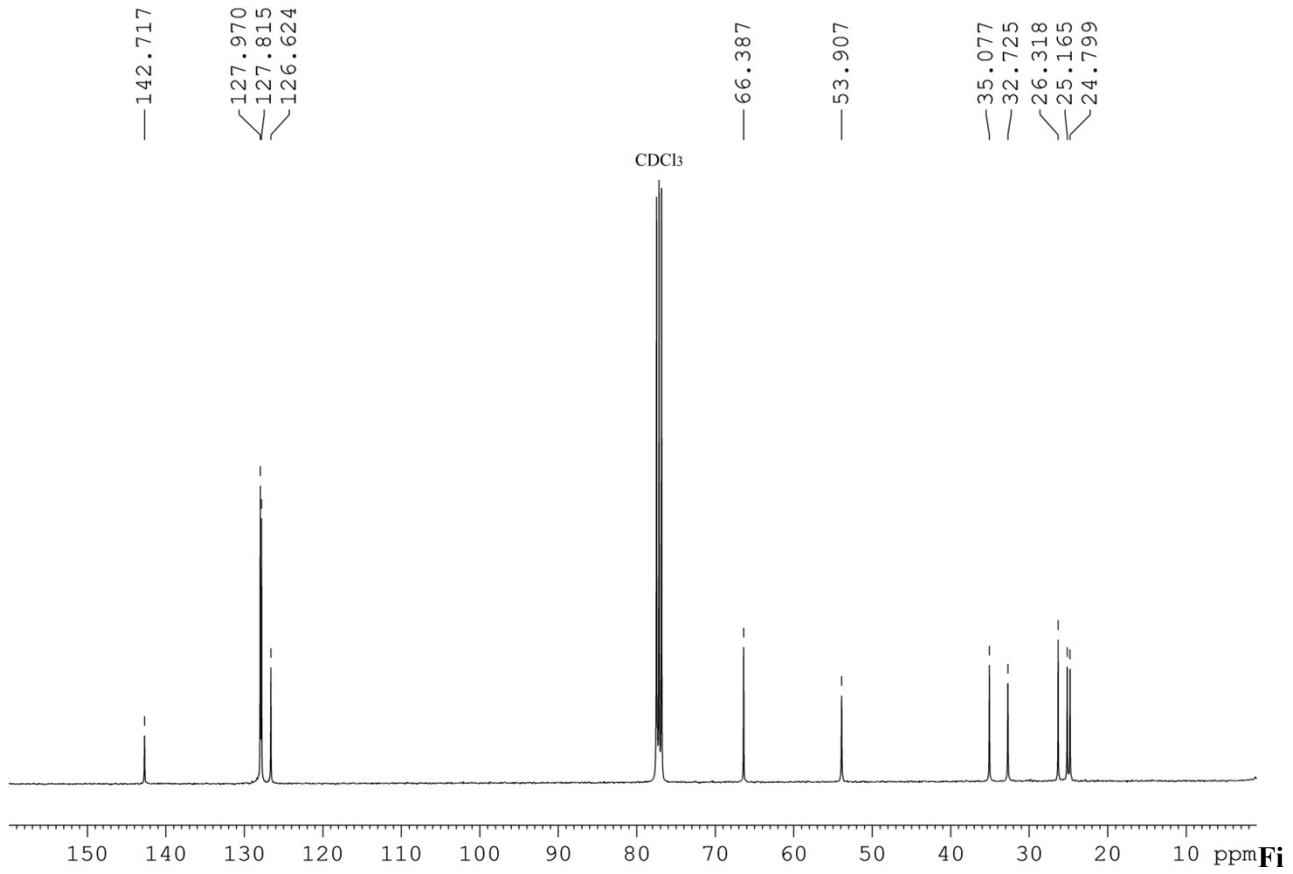

Figure S8: ^{13}C{H}NMR of **D** ($CDCl_3$, 100 MHz).

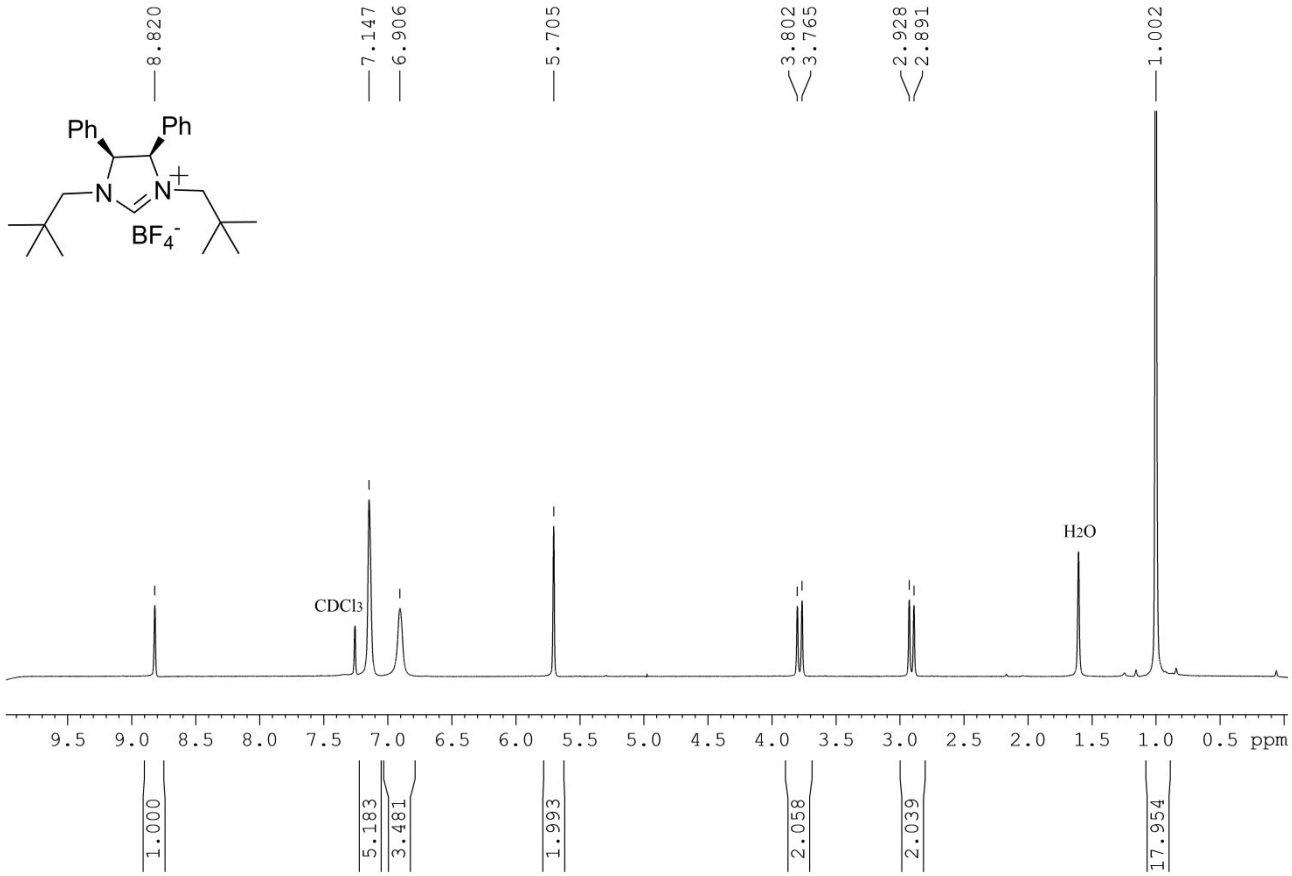

Figure S9: ^{1}H NMR of **E** ($CDCl_3$, 400 MHz).

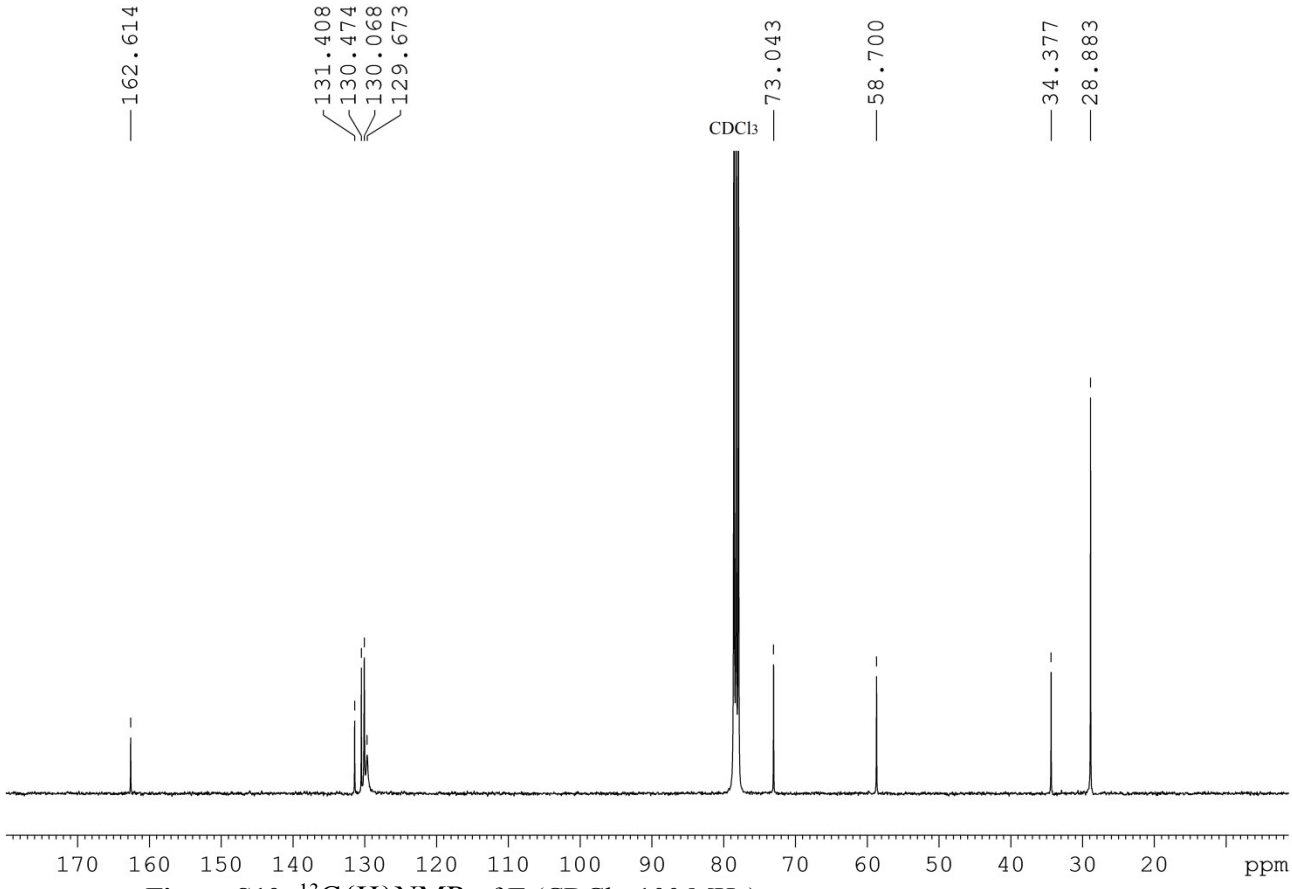

Figure S10: ^{13}C{H}NMR of **E** ($CDCl_3$, 100 MHz).

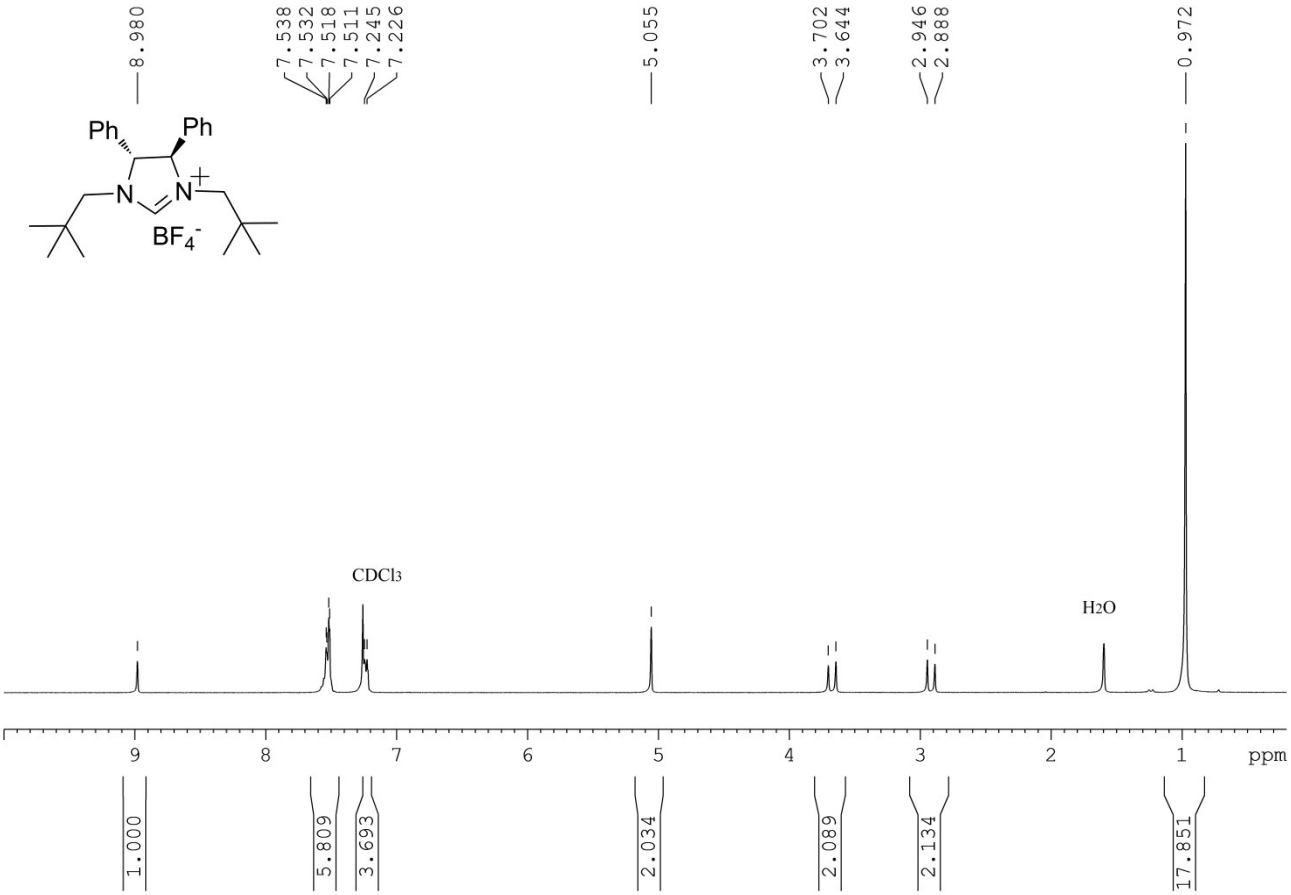

Figure S11: ^{1}H NMR of **F** ($CDCl_3$, 250 MHz).

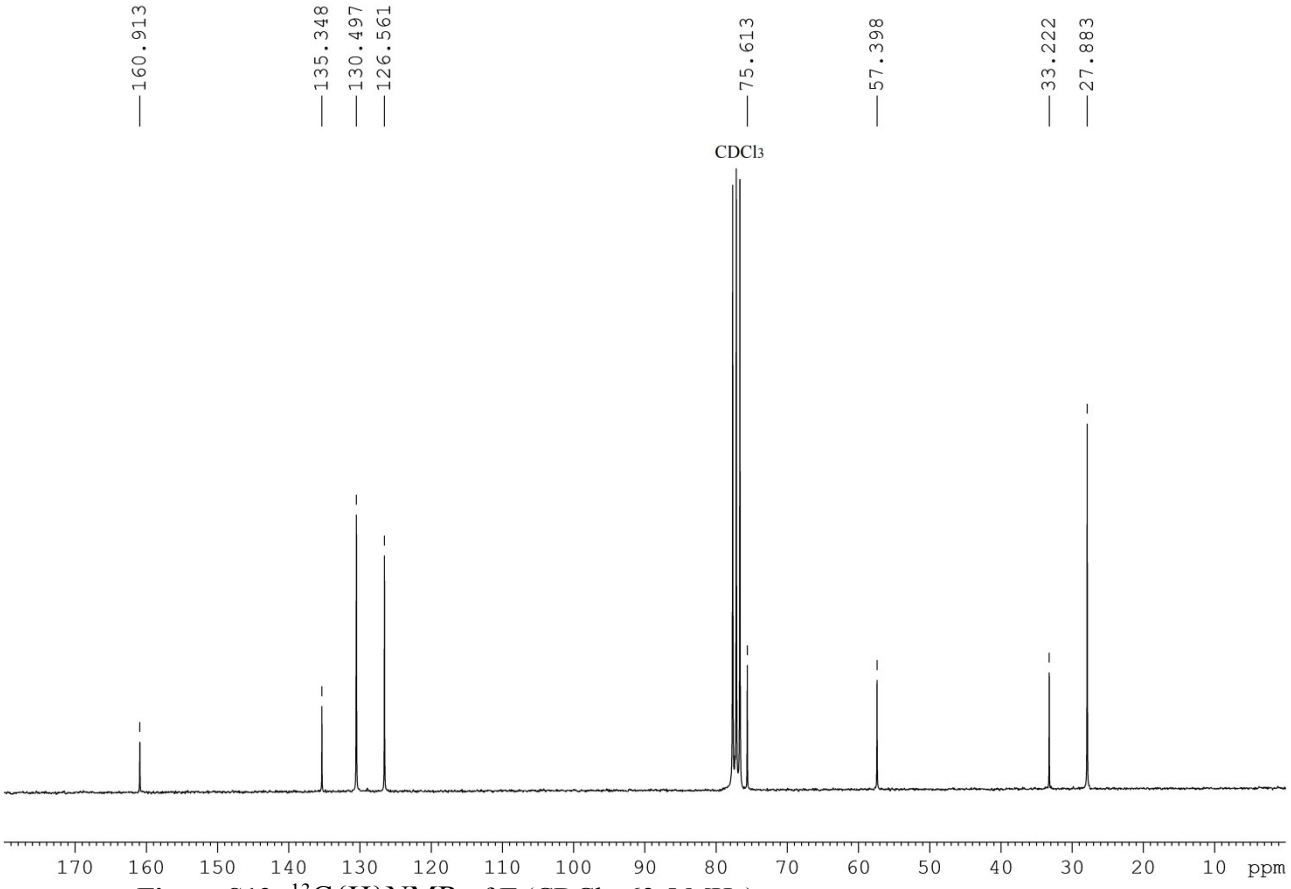

Figure S12: ^{13}C{H}NMR of **F** ($CDCl_3$, 62.5 MHz).

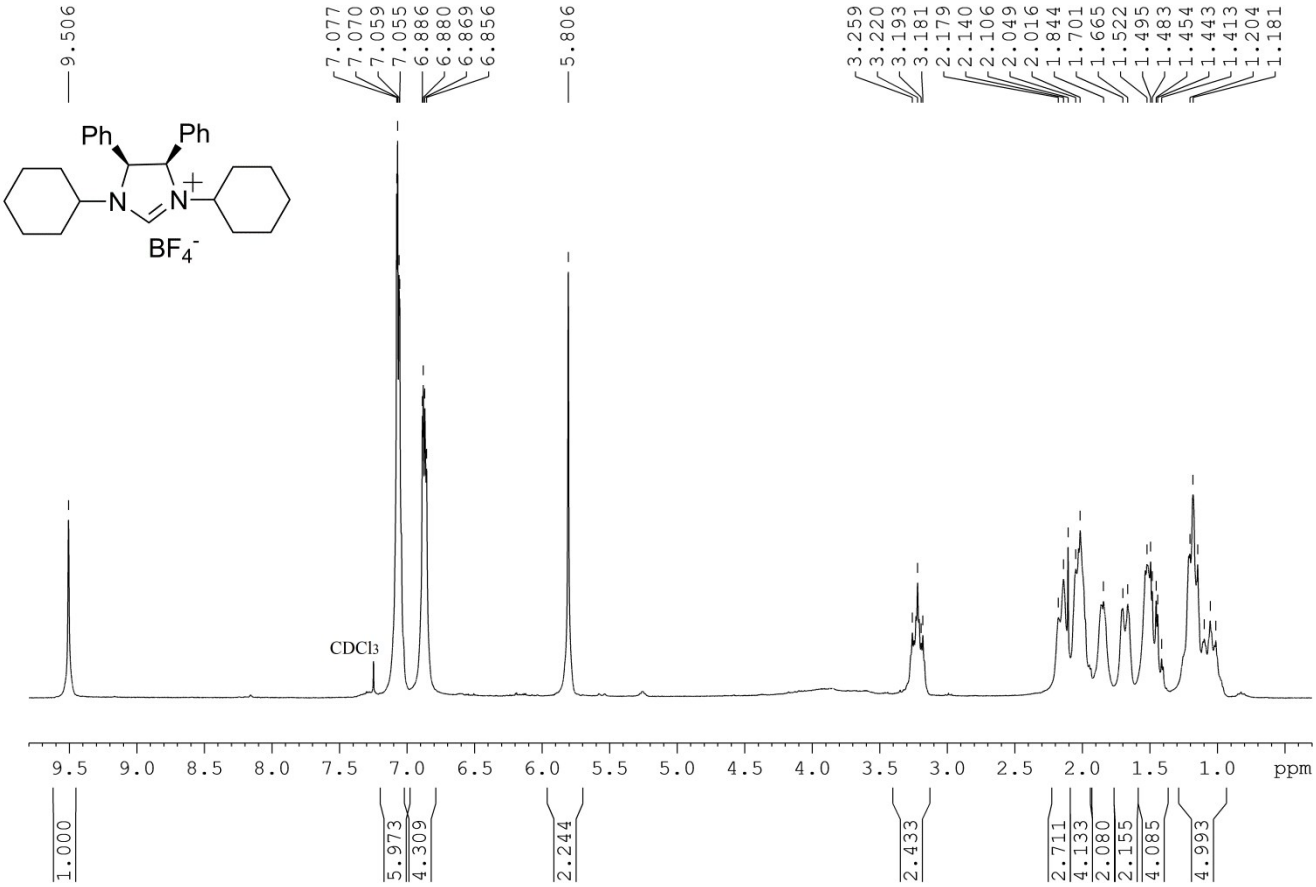

Figure S13: ^{1}H NMR of **G** ($CDCl_3$, 300 MHz).

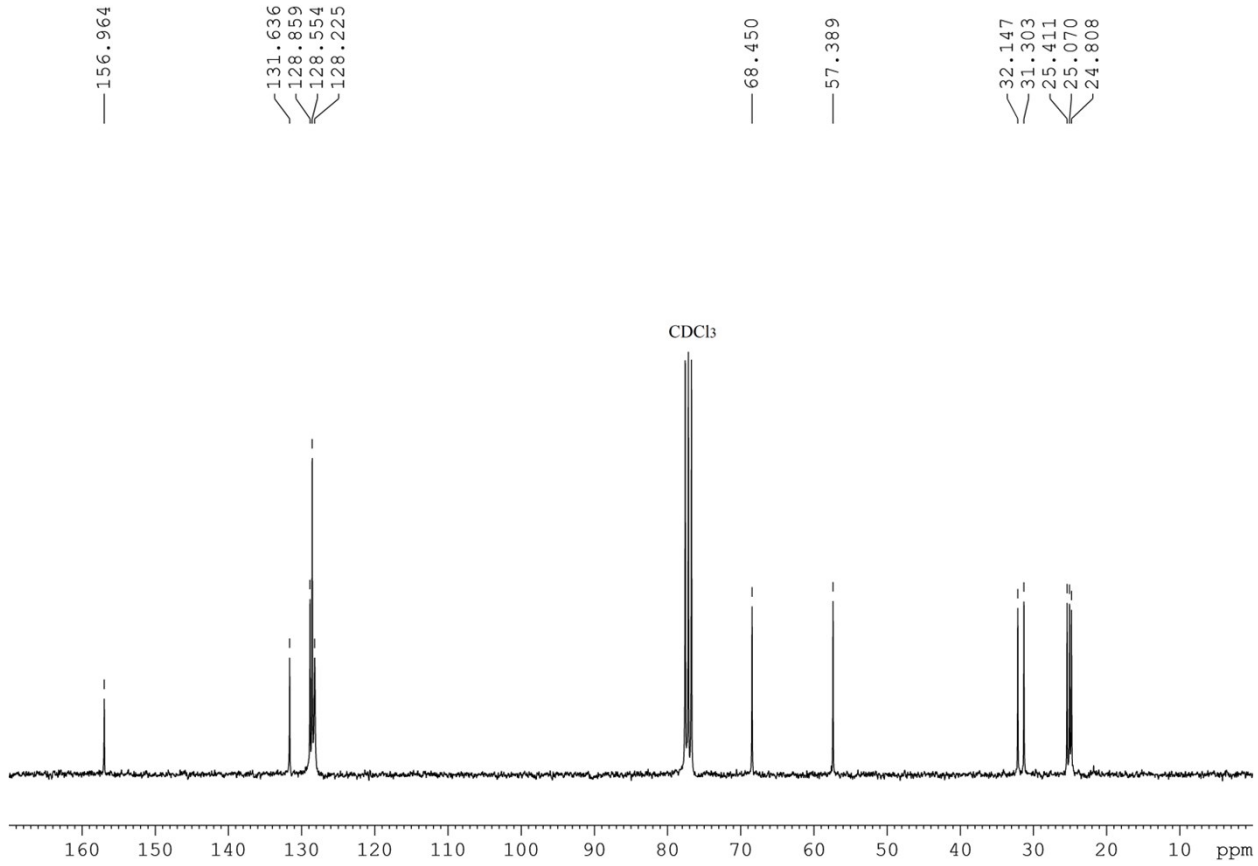

Figure S14: ^{13}C{H}NMR of **G** ($CDCl_3$, 75 MHz).

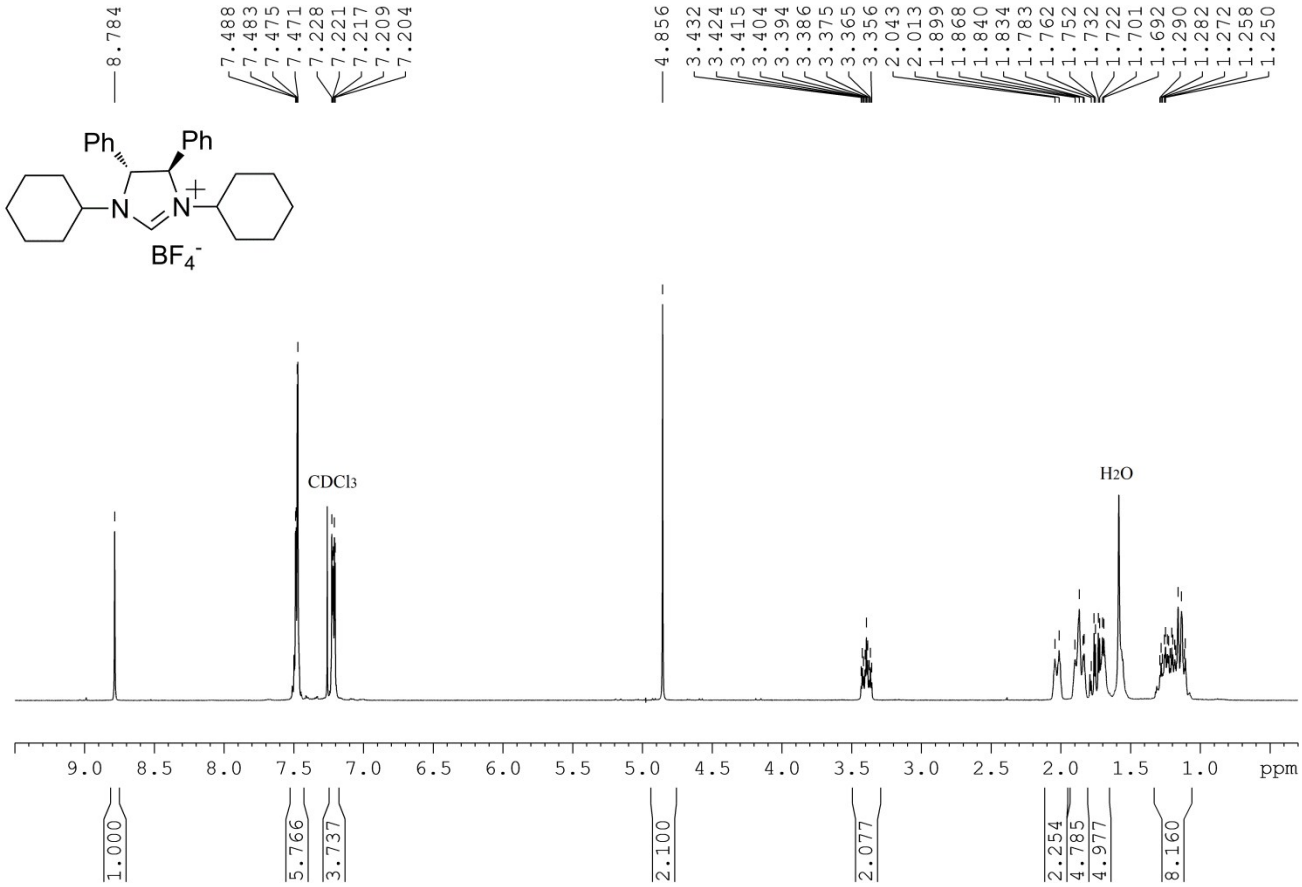

Figure S15: ^{1}H NMR of **H** ($CDCl_3$, 400 MHz).

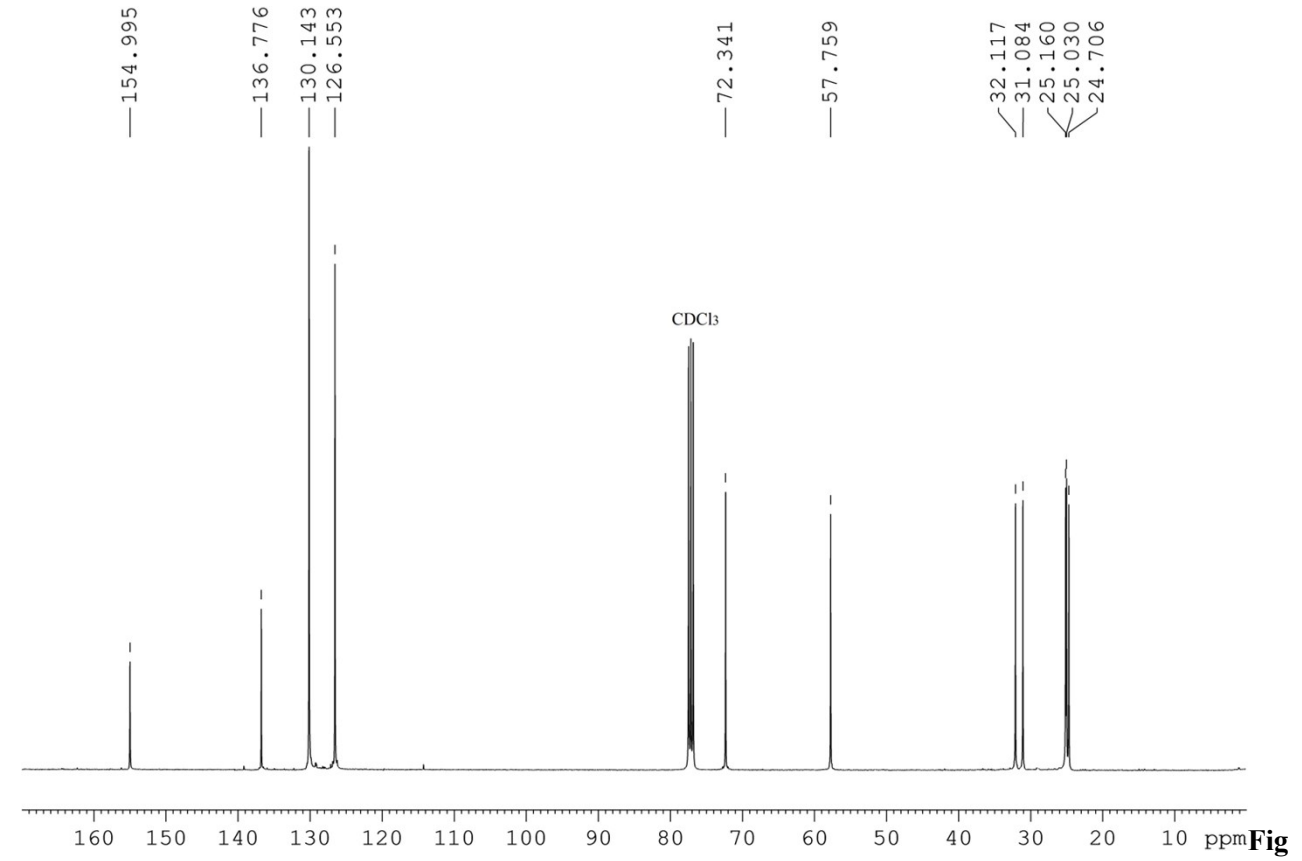

Figure S16: ^{13}C{H}NMR of **H** ($CDCl_3$, 100 MHz).

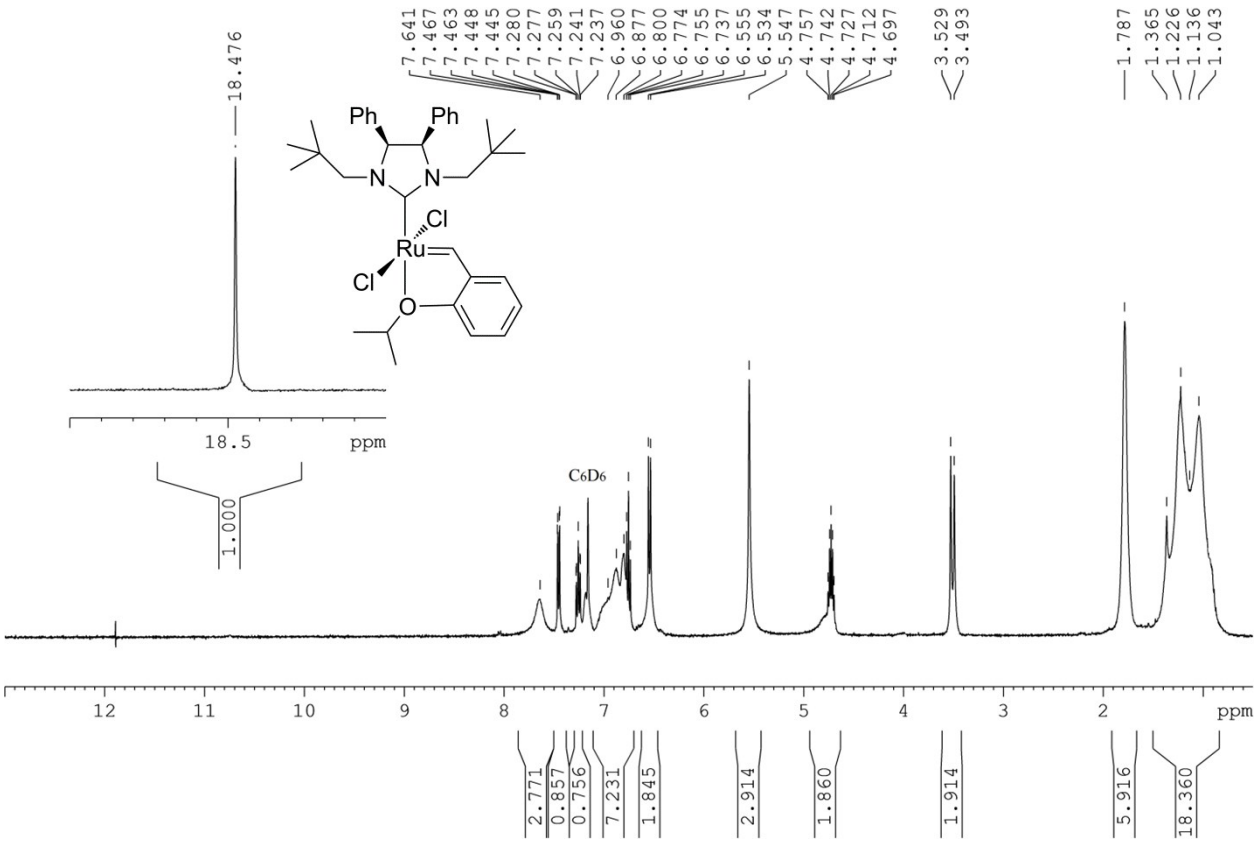

Figure S17: ^{1}H NMR of **4** (C_6D_6, 400 MHz).

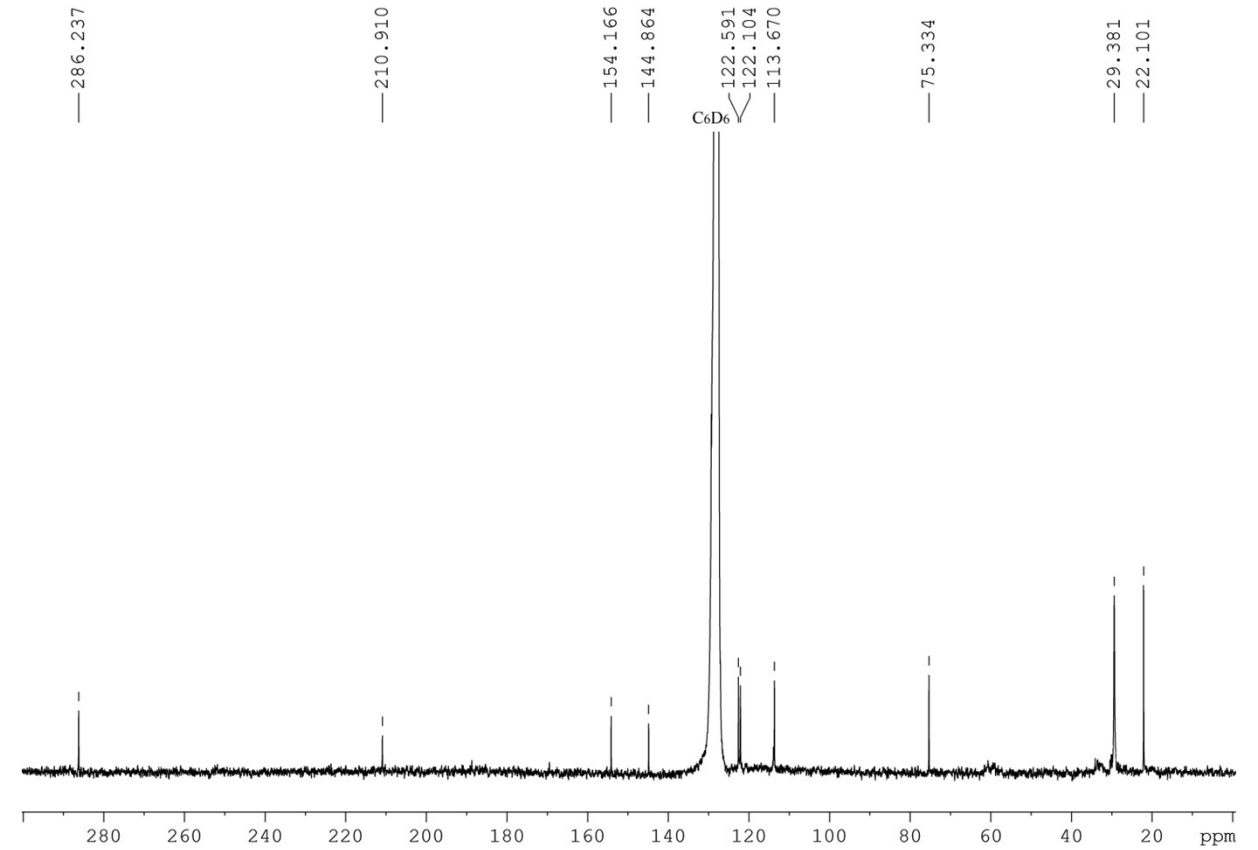

Figure S18: ^{13}C{H}NMR of **4** (C_6D_6, 75 MHz).

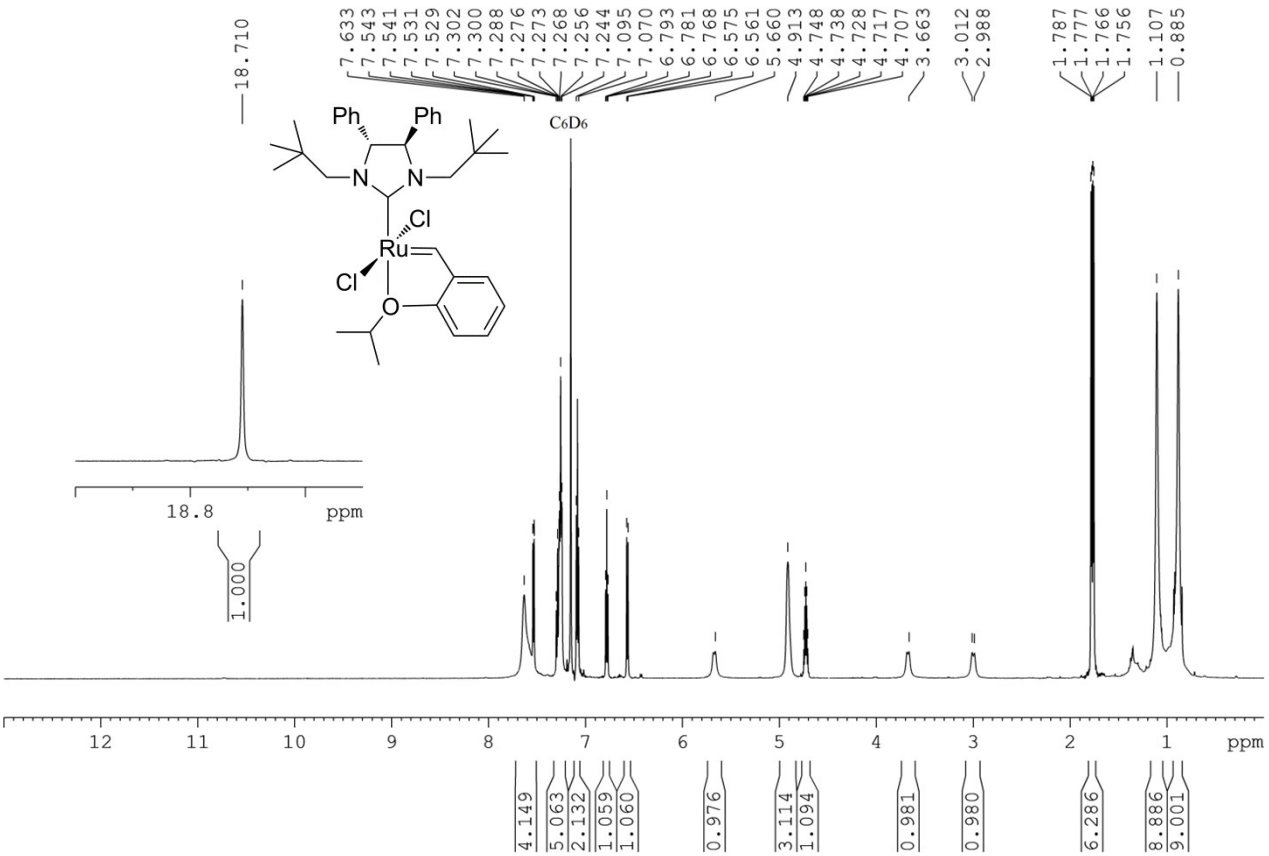

Figure S19: ^{1}H NMR of **5** (C_6D_6, 600 MHz).

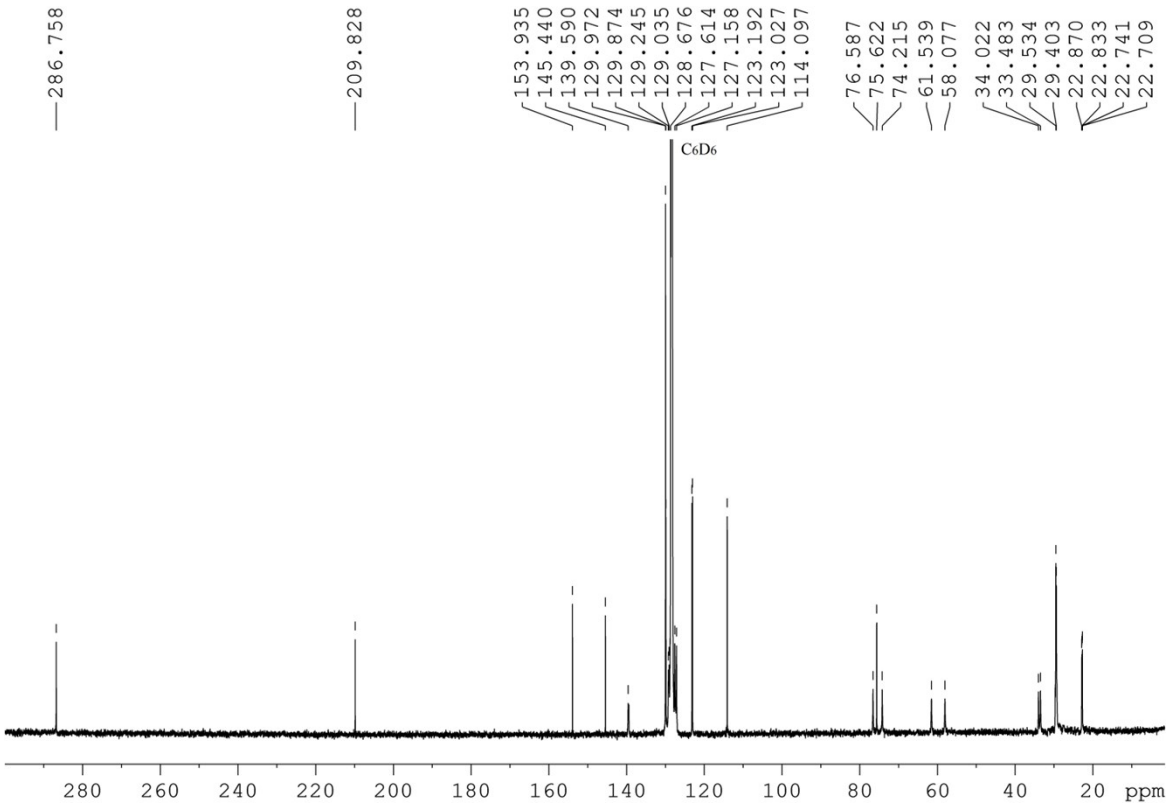

Figure S20: ^{13}C{H}NMR of **5** (C_6D_6, 125 MHz).

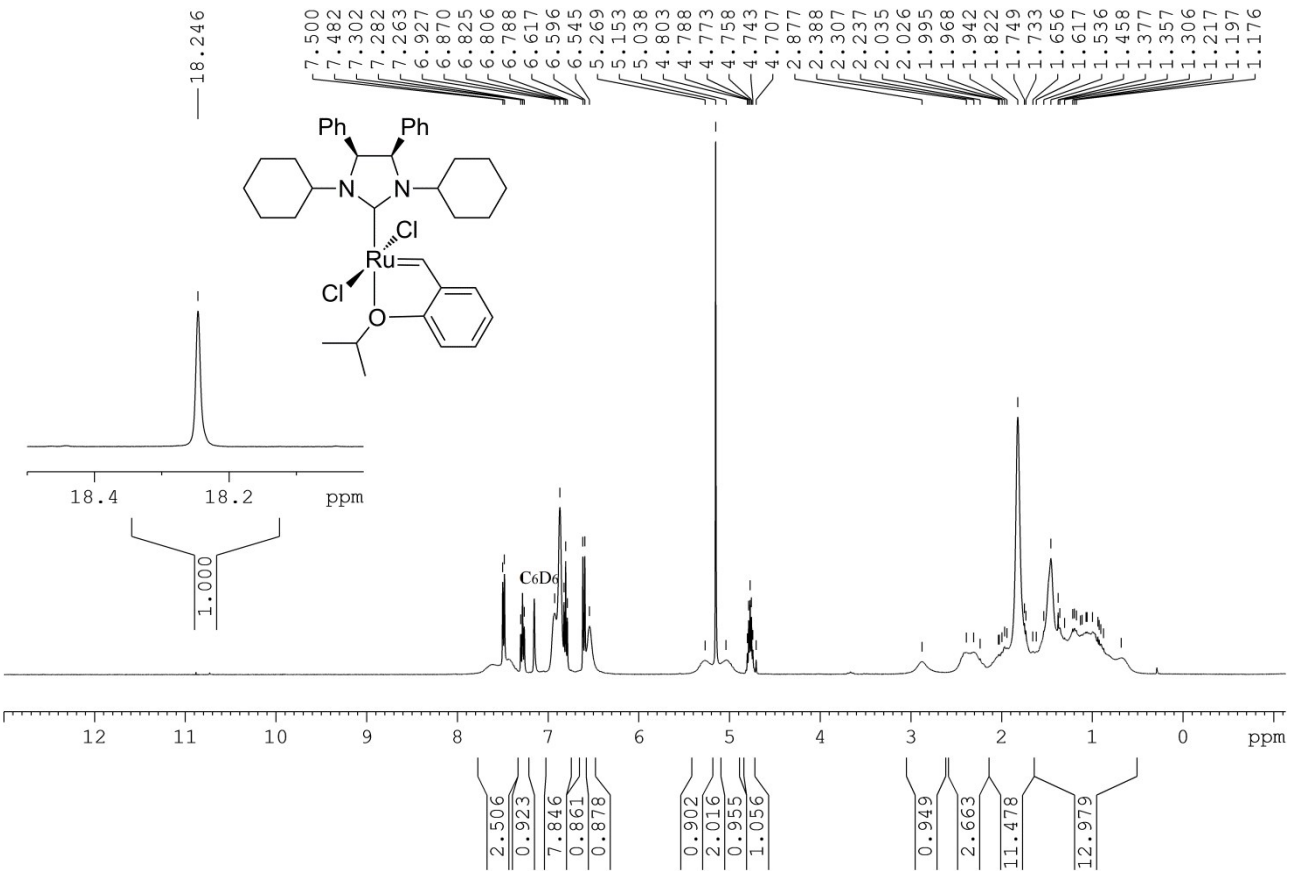

Figure S21: ^{1}H NMR of **6** (C_6D_6, 400 MHz).

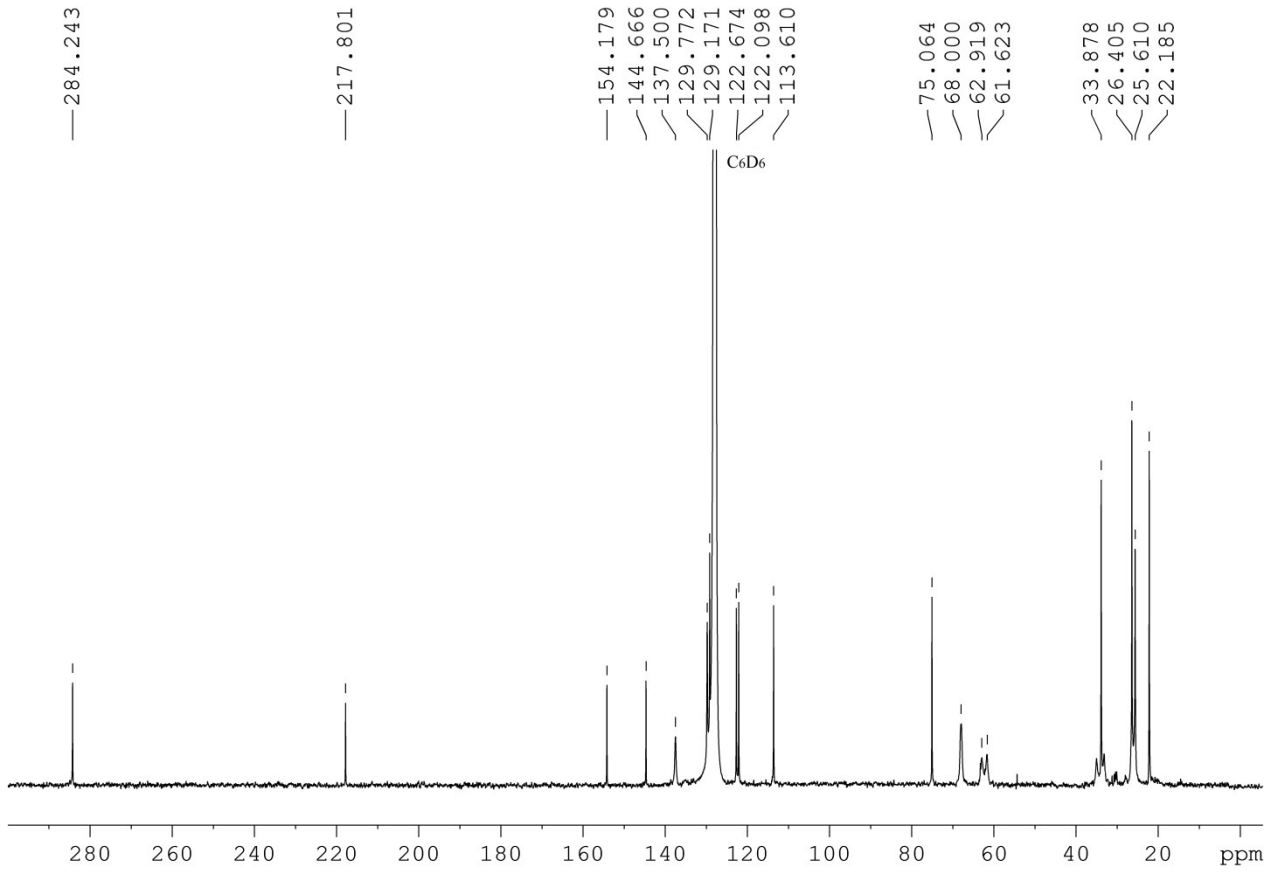

Figure S22: ^{13}C{H}NMR of **6** (C_6D_6, 100 MHz).

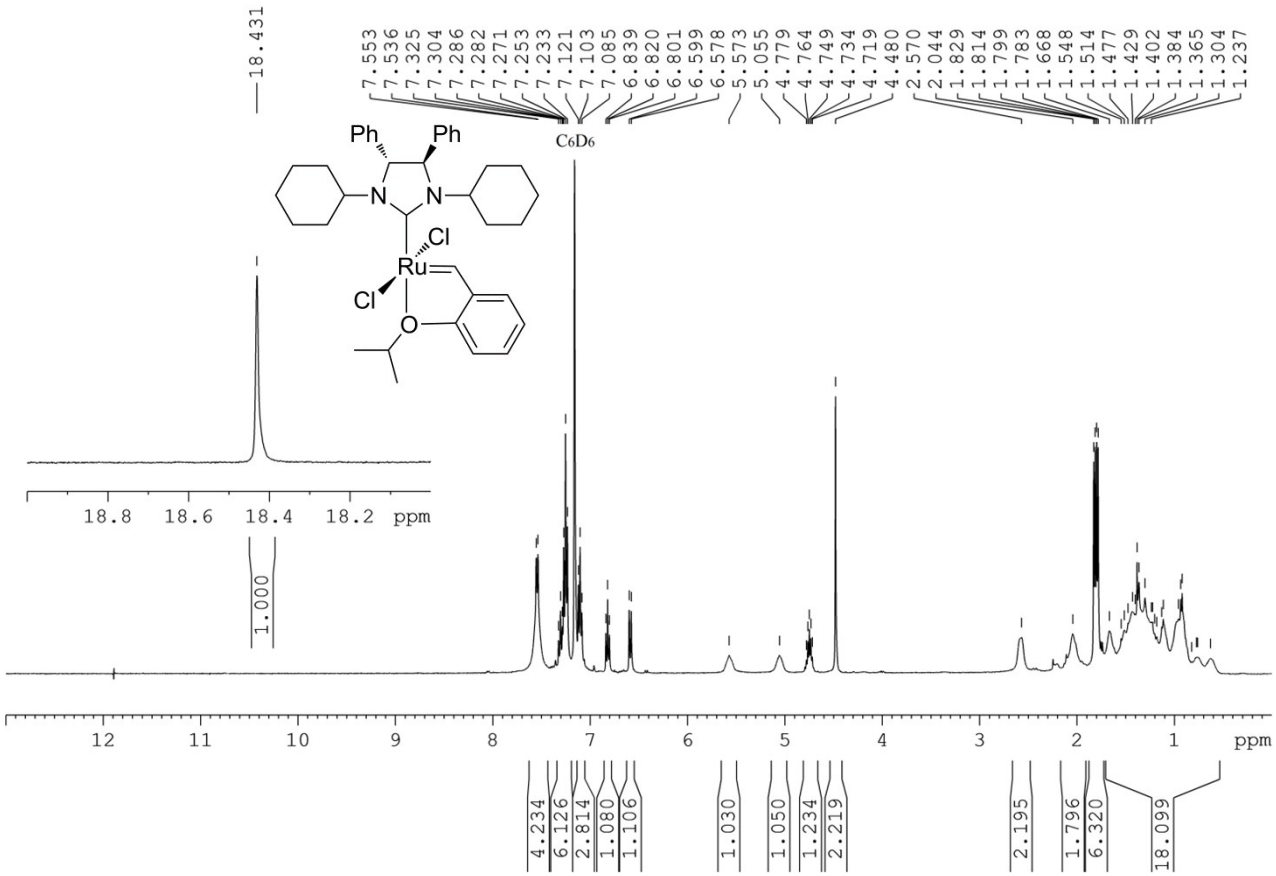

Figure S23: ^{1}H NMR of **7** (C_6D_6, 400 MHz).

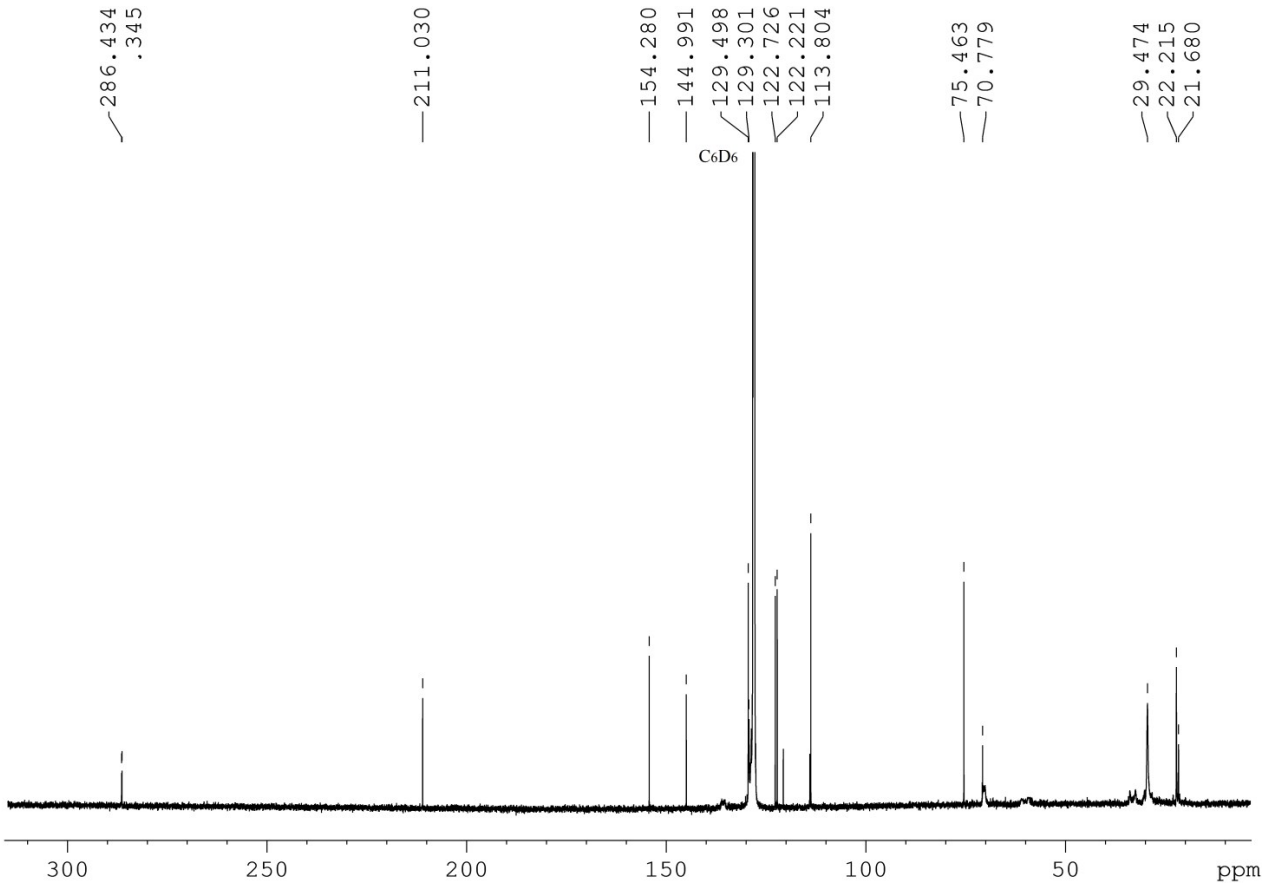

Figure S24: ^{13}C{H}NMR of **7** (C_6D_6, 125 MHz).

ESI-FT-ICR spectra

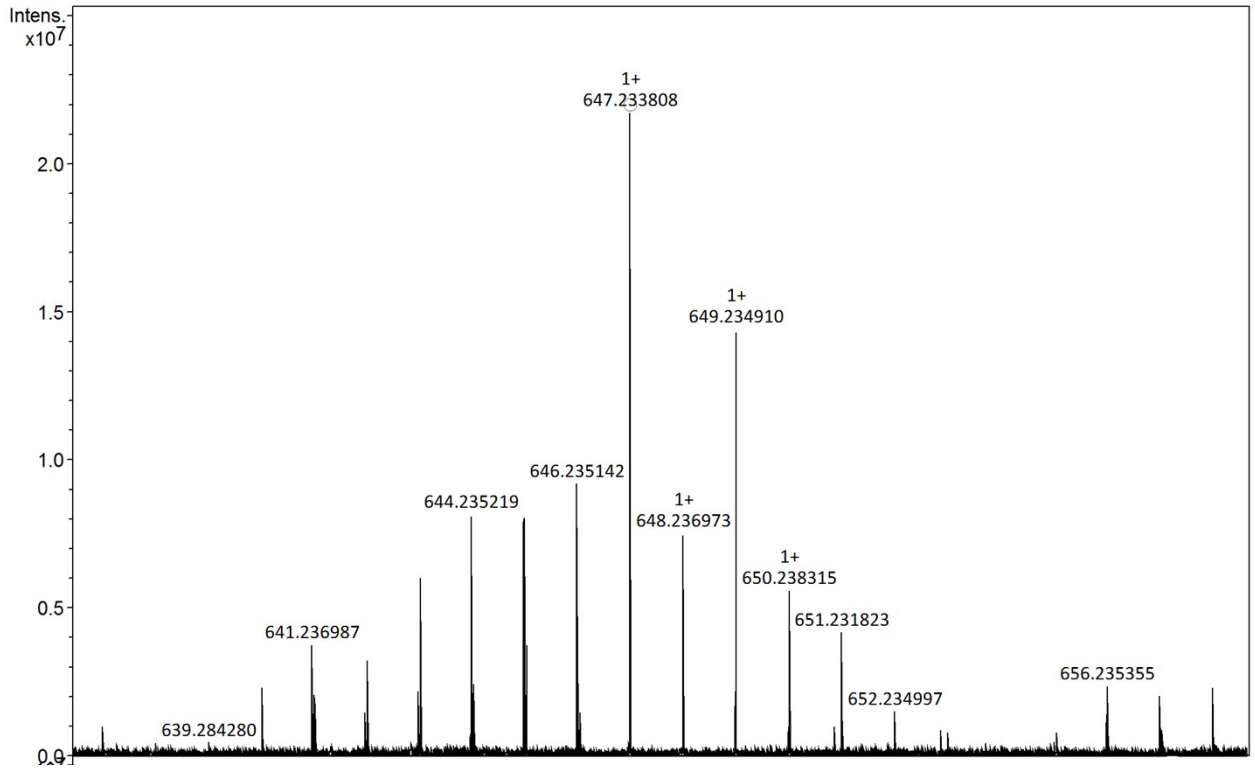

Figure S25. ESI-FT-ICR of **4**

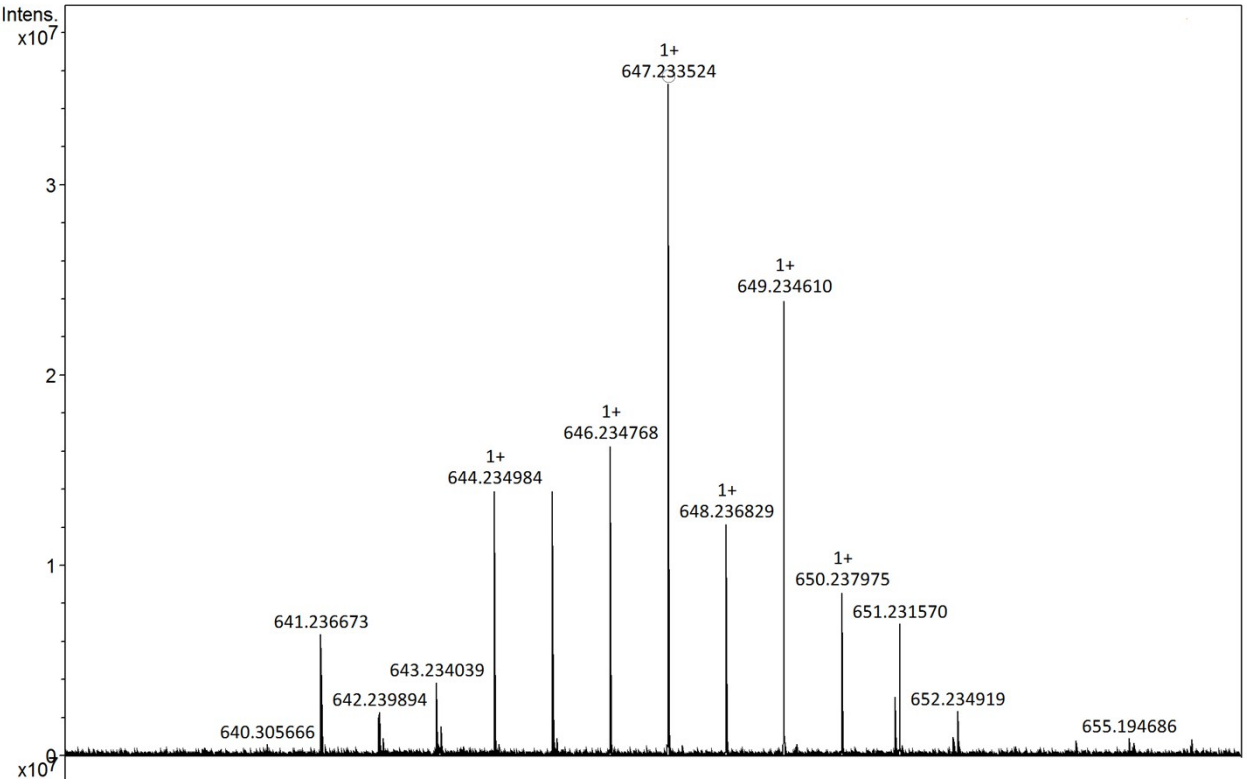

Figure S26. ESI-FT-ICR of **5**

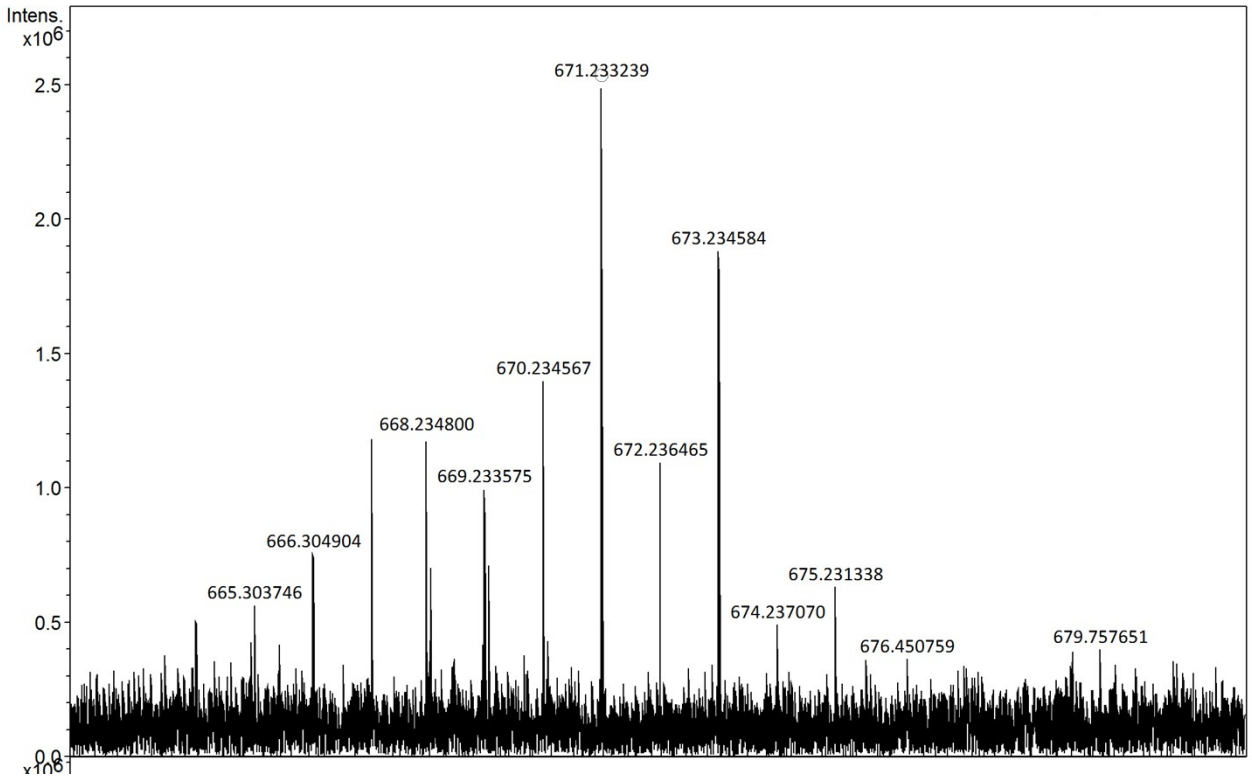

Figure S27. ESI-FT-ICR of **6**

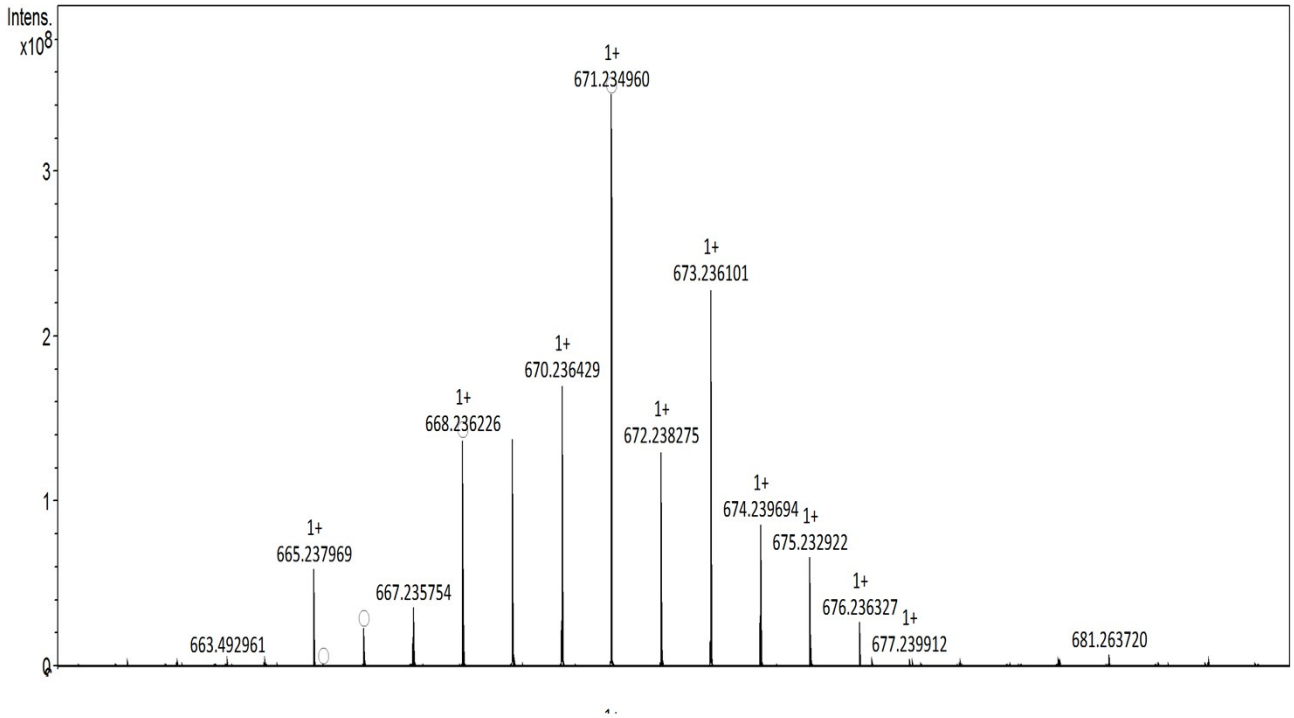

Figure S28. ESI-FT-ICR of **7**

Crystal structure determination

The crystal data of compound **6** were collected at room temperature using a Nonius Kappa CCD diffractometer with graphite monochromated Mo-Kα radiation. The data set was integrated with the Denzo-SMN package[1] and corrected for Lorentz, polarization and absorption effects (SORTAV). [2] The structure was solved by direct methods using SIR97[3] system of programs and refined using full-matrix least-squares with all non-hydrogen atoms anisotropically and hydrogens included on calculated positions, riding on their carrier atoms.

Ill-defined regions of residual eletron density were found, occupied probably by disordered solvent molecules of pentane and diethyl ether, which can not be localized. For these reasons the program SQUEEZE was used to cancel out mathematically the effects of the disordered solvent, treated as a diffuse contribution to the overall scattering without specific atom positions. SQUEEZE is part of the PLATON[4] program system.

All calculations were performed using SHELXL-2014/6[5] and PARST[6] implemented in WINGX[7] system of programs. The crystal data are given in Table S1. A selection of bond distances and angles is given in Table S2.

Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition numbers CCDC 1564122. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html or on application to CCDC, Union Road, Cambridge, CB2 1EZ, UK [fax: (+44)1223-336033, e-mail: deposit@ccdc.cam.ac.uk]

[1] Z. Otwinowski, W. Minor, *Methods in Enzymology*, C.W. Carter, R.M. Sweet Editors, Vol. 276, Part A, Academic Press, London, 1997, 307.
[2] R. H. Blessing, *Acta Crystallogr.,*1995, **A51**, 33.
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[4] A. L. Spek, *Acta Crystallogr.,* **2009**, **D65**, 148.
[5] G. M. Sheldrick, *Crystal Structure Refinement with SHELXL*, *Acta. Crystallogr*., 2015, **C71**, 3.
[6] M. Nardelli, *J. Appl. Crystallogr*., 1995, **28**, 659.
[7] L. J. Farrugia, *J. Appl. Crystallogr*., 1999, **32**, 837.

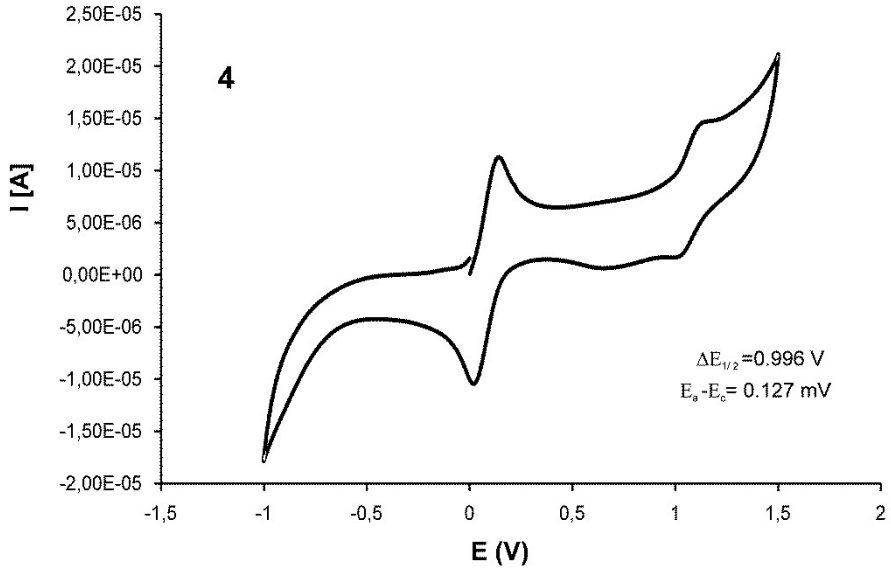
Table S1. Crystallographic data.

Compound	**6**
Formula	$C_{37}H_{46}Cl_2N_2ORu$
M	706.73
Space group	$P2_1/c$
Crystal system	Monoclinic
a/Å	10.6467(1)
b/Å	22.5668(5)
c/Å	15.5514(4)
β/°	93.659(1)
U/Å^3	3728.8(1)
Z	4
T/K	295
D_c/g cm^{-3}	1.259
F(000)	1472
μ(Mo-Kα)/mm^{-1}	0.592
Measured Reflections	34036
Unique Reflections	10835
R_{int}	0.0547
Obs. Refl.ns [I≥2σ(I)]	7684
θ_{min}- θ_{max}/°	3.32 – 30.00
hkl ranges	-14,14;-31,30;-14,21
R(F^2) (Obs.Refl.ns)	0.0367
wR(F^2) (All Refl.ns)	0.0930
No. Variables/Restraints	390/0
Goodness of fit	1.012
$\Delta\rho_{max}$; $\Delta\rho_{min}$ /e Å^{-3}	0.338; -0.717
CCDC Dep. N.	1564122

Table S2. Selected bond distances and angles (Å and degrees)

Distances	**6**
Ru1-Cl1	2.3286(5)
Ru1-Cl2	2.3595(6)
Ru1-C1	1.975(2)
Ru1-C4	1.828(2)
Ru1-O1	2.291(1)
C1-N1	1.354(2)
C1-N2	1.351(2)
Angles	
Cl1-Ru1-Cl2	156.54(2)
Cl1-Ru1-C1	90.38(5)
Cl1-Ru1-C4	101.72(6)
Cl1-Ru1-O1	86.79(4)
Cl2-Ru1-C1	93.13(5)
Cl2-Ru1-C4	100.40(6)
Cl2-Ru1-O1	89.97(4)
C1-Ru1-C4	100.73(8)
C1-Ru1-O1	176.90(6)
C4-Ru1-O1	78.63(7)
Ru1-C1-N1	119.14(13)
Ru1-C1-N2	131.83(12)
N1-C1-N2	108.98(15)

Cyclic Voltammograms



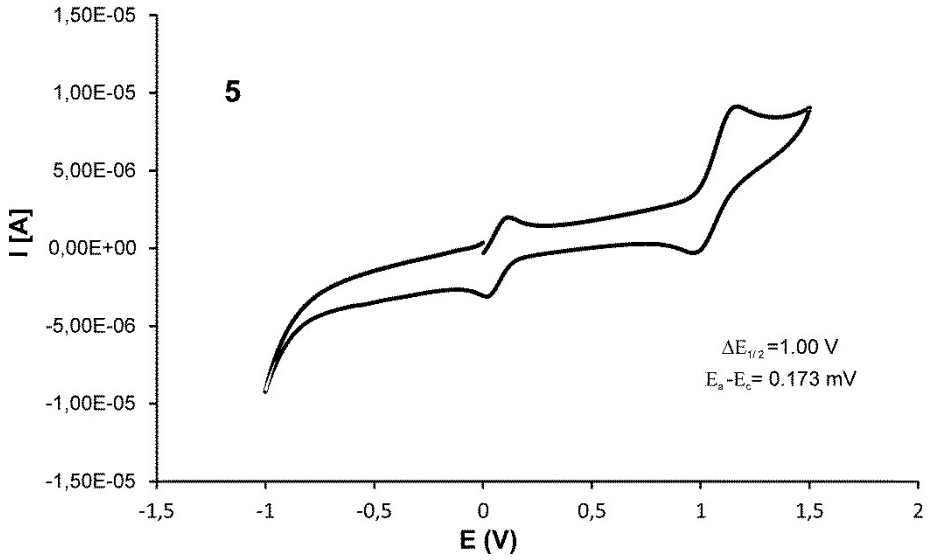


Figure S29. Cyclic voltammograms of **4** and **5**

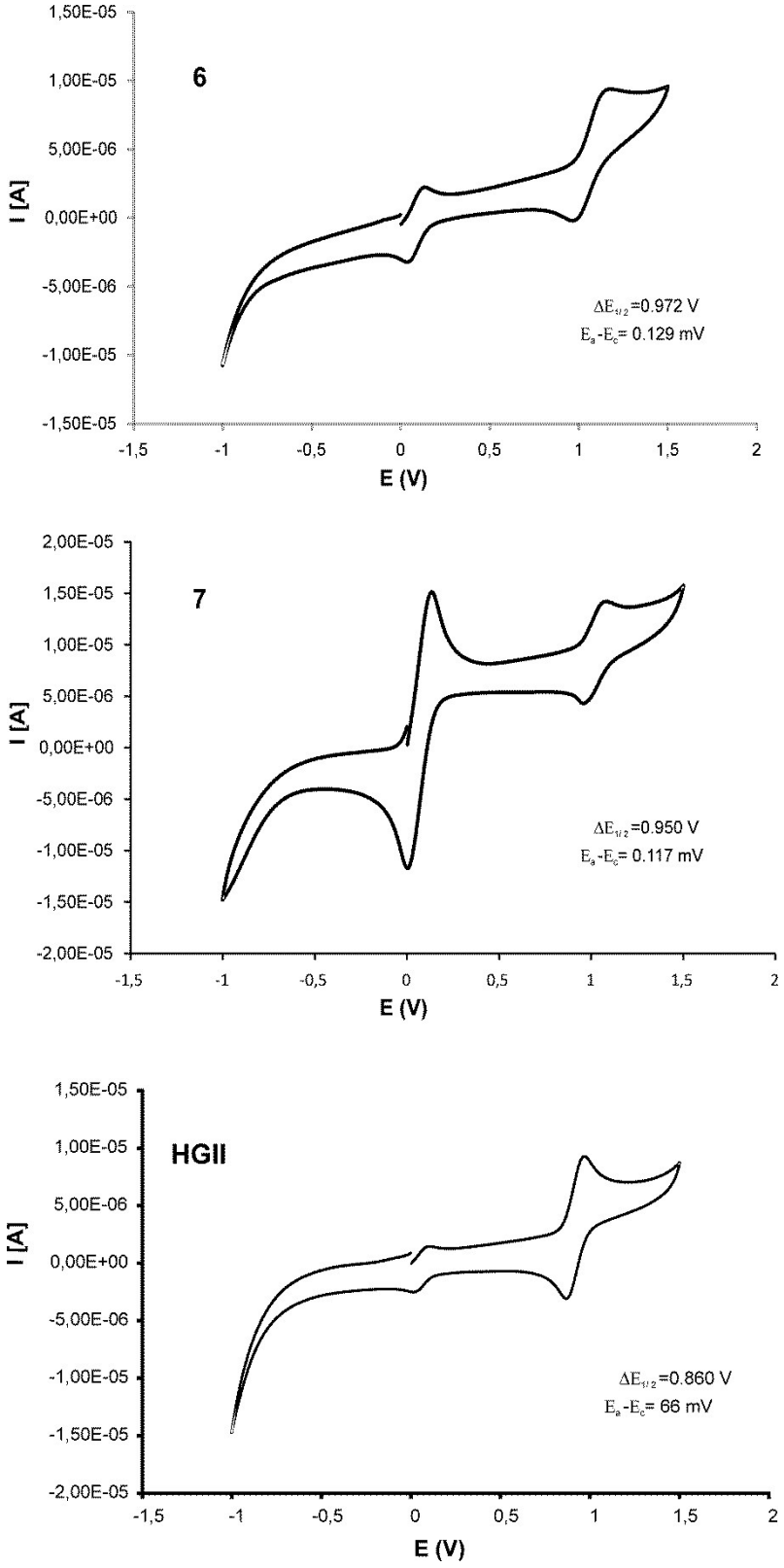
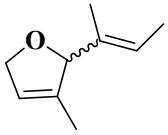


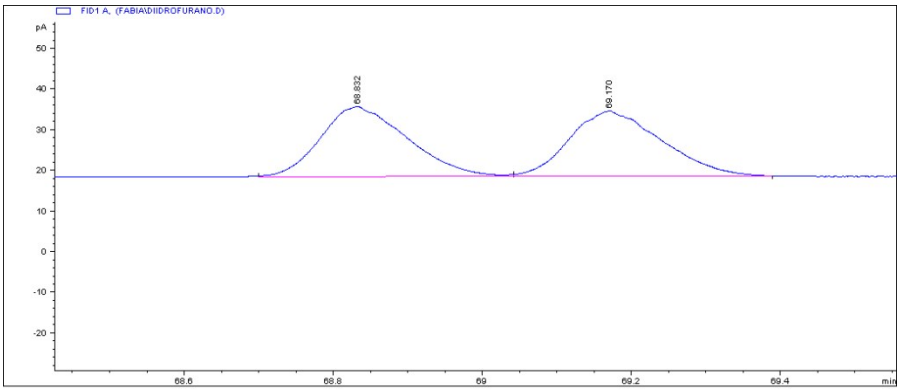
Figure S30. Cyclic voltammograms of **6, 7** and **HGII**

GC data analysis

Supelco β-DEX 120, 1mL/min, 40°C for 100min, then 1°C/ min up to 50°C for 120 min, then 1°C/ min up to 100°C for 10 min.



Racemic



36% *ee*

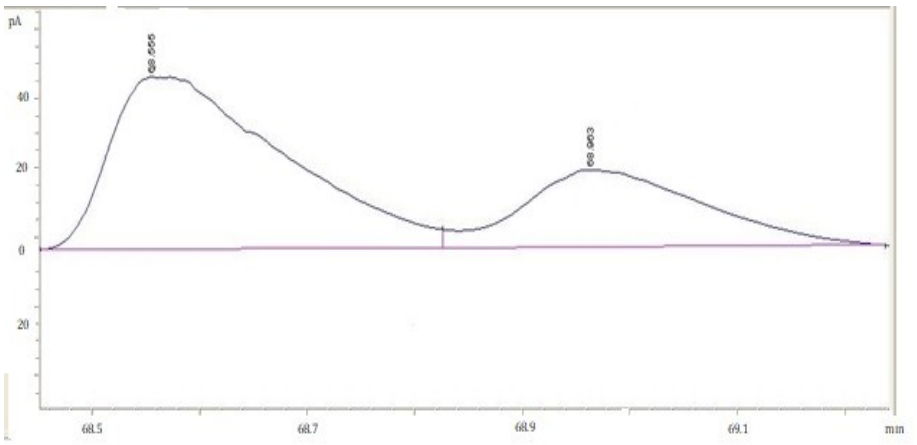
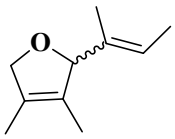
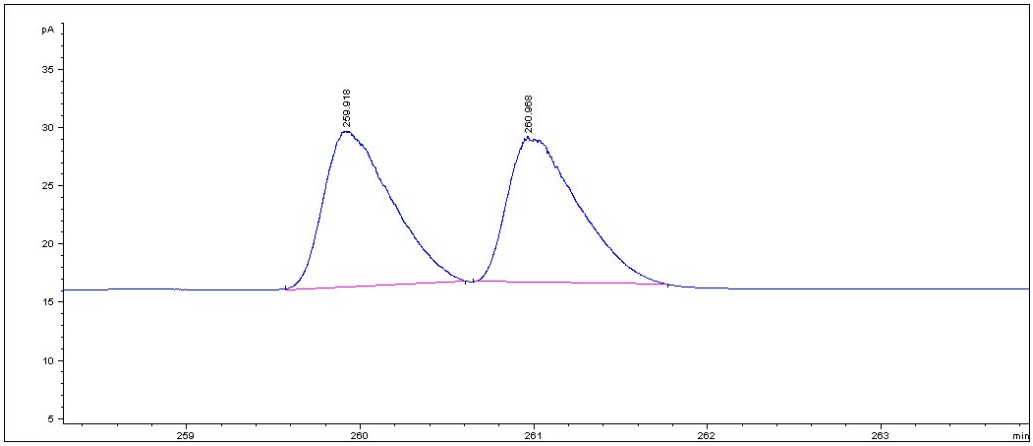


Figure S31: GC chromatogram of **29** obtained with catalyst **5**

Supelco β-DEX 120, 1mL/min, 40°C for 100min, then 1°C/ min up to 50°C for 120 min, then 1°C/ min up to 100°C for 10 min.



Racemic



33%*ee*

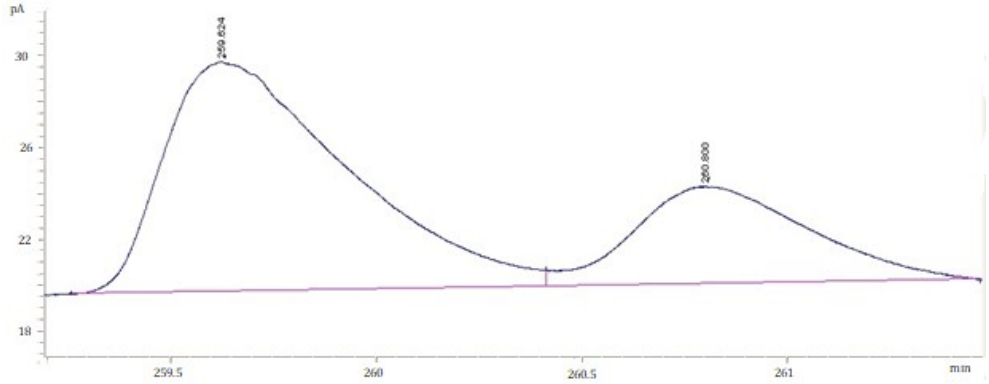


Figure S32: GC chromatogram of **31** obtained with catalyst **7**

Cartesian coordinates and energies of calculated structures

Computational details relative to calculations on Hoveyda-Grubbs' catalysts and* BDE *of NHC

The DFT calculations were performed with the Gaussian09 set of programs,[8] using the PBE0 model.[9] The electronic configuration of the molecular systems was described with 6-311G(d,p) basis set for H, C, N, O, and Cl.[10] For Ru we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated (8s7p6d)/[6s5p3d] valence basis set contracted according to a (311111/22111/411) scheme (standard SDD keywords in gaussian09).[11] The geometry optimizations were performed without symmetry constraints.

%V_{Bur} calculation. %V_{Bur} was calculated with the software developed by Cavallo and coworkers[12], starting from DFT optimized structures by choosing the metal as center of the sphere, selecting atomic bondi radii scaled by 1.17 and radius sphere of 3.5.

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HGII SCF Done: -2402.71052963 A.U.

Ru	-0.182892	0.462902	-0.040624
Cl	-0.522009	0.564557	-2.364289
Cl	-0.682147	0.665801	2.248715
C	-0.147435	-1.504860	-0.001677
N	0.854626	-2.410489	0.026709
C	0.390904	-3.799194	0.063209
H	0.720038	-4.283797	0.988115
C	-1.127131	-3.655457	-0.018594
H	-1.641674	-4.108887	0.833943
N	-1.309275	-2.207392	-0.011437
H	0.809827	-4.361391	-0.776494
H	-1.542395	-4.085952	-0.935766
C	2.256397	-2.172189	0.065286
C	2.894996	-2.052462	1.305208
C	4.273248	-1.852008	1.315572
H	4.778478	-1.743710	2.271736
C	5.014303	-1.774558	0.138284
C	6.504169	-1.590243	0.179022
C	4.343096	-1.895783	-1.076368
H	4.903155	-1.823164	-2.004928
C	2.966294	-2.097866	-1.138472
C	2.255301	-2.169206	-2.456748
C	2.110418	-2.072892	2.583364
H	1.370656	-1.265673	2.603876
H	2.772454	-1.953977	3.443017
H	1.566028	-3.014388	2.710788
C	-2.625318	-1.653635	-0.030611
C	-3.296612	-1.435604	1.183377
C	-4.566026	-0.865448	1.141785
H	-5.079444	-0.670927	2.079861
C	-5.194102	-0.551348	-0.059429
C	-6.538617	0.115944	-0.075353
C	-4.542361	-0.872936	-1.245771
H	-5.037221	-0.685151	-2.195166
C	-3.272321	-1.443607	-1.259058
C	-2.686052	-1.899075	-2.562582
C	-2.733446	-1.880604	2.500634
H	-3.155195	-2.857490	2.768971
H	-2.993882	-1.176266	3.292265
H	-1.648251	-1.957963	2.481221
C	1.591223	0.865653	-0.008739
H	2.405492	0.144722	0.061528
C	2.003730	2.247296	-0.100655
C	3.348234	2.631262	-0.156880
H	4.108524	1.857010	-0.114862
C	3.700894	3.966528	-0.269417
H	4.744418	4.257184	-0.313903
C	2.702272	4.933173	-0.326949
H	2.969034	5.981066	-0.417744
C	1.355351	4.585849	-0.267936
H	0.599230	5.358991	-0.311022
C	1.012728	3.245767	-0.153253
O	-0.249078	2.755216	-0.094267
C	-1.394873	3.641967	-0.003941
H	-1.245416	4.422242	-0.758988
C	-1.486870	4.235591	1.388601
H	-1.621221	3.435155	2.119387

H	-2.343119	4.914515	1.438663
H	-0.589878	4.797895	1.656490
C	-2.609989	2.822061	-0.374868
H	-2.481728	2.359518	-1.355089
H	-3.486800	3.475275	-0.400865
H	-2.789781	2.038965	0.368244
H	-2.922582	-1.195196	-3.362195
H	-1.602234	-1.986519	-2.521905
H	-3.112730	-2.872375	-2.835775
H	2.967304	-2.113806	-3.282278
H	1.691766	-3.101916	-2.563309
H	1.539572	-1.346663	-2.561180
H	6.867454	-1.076189	-0.714033
H	6.811029	-1.013479	1.054889
H	7.014063	-2.558718	0.229747
H	-7.120814	-0.178865	-0.951907
H	-7.116949	-0.128739	0.818826
H	-6.428538	1.205648	-0.106943

87

4 hov-npnt-syn SCF Done: -2559.78583260 A.U.

Ru	-1.549239	-0.188526	0.015487
Cl	-2.115754	-0.483840	2.276892
Cl	-1.030456	-0.916263	-2.152860
N	1.096556	-0.975846	0.746286
N	1.229016	1.155246	0.278615
C	0.373029	0.116576	0.387038
C	2.537128	-0.753910	0.672924
H	3.021442	-1.132588	1.575929
C	2.582104	0.796727	0.723669
H	2.682576	1.081485	1.779379
C	-2.256463	1.471568	-0.217353
H	-1.718797	2.413539	-0.108366
C	-3.664739	1.629647	-0.498821
C	-4.276864	2.882708	-0.617397
H	-3.665435	3.773350	-0.507882
C	-5.635398	2.989771	-0.865506
H	-6.102067	3.964085	-0.955061
C	-6.396666	1.833236	-0.997200
H	-7.461887	1.906239	-1.190140
C	-5.818999	0.571511	-0.887450
H	-6.436035	-0.310575	-0.997124
C	-4.456634	0.475279	-0.638296
C	-4.400873	-1.958703	-0.715883
H	-5.367679	-1.917815	-0.201924
C	-3.540930	-3.010036	-0.053523
H	-2.579645	-3.097250	-0.567647
H	-4.048217	-3.976818	-0.113053
H	-3.369934	-2.763368	0.995906
C	-4.578624	-2.194417	-2.203346
H	-5.183571	-1.416179	-2.673517
H	-5.075174	-3.155807	-2.363301
H	-3.601369	-2.211872	-2.690910
O	-3.758941	-0.676725	-0.486970
C	0.530986	-2.312453	0.830365
H	0.767161	-2.877016	-0.080201
H	-0.556953	-2.190229	0.858557
C	0.907490	-3.159534	2.070691
C	2.232645	-3.902148	1.868587
H	2.426628	-4.554611	2.726210

H	3.088746	-3.231630	1.767592
H	2.200042	-4.528541	0.971482
C	-0.202830	-4.208001	2.212681
H	-0.319670	-4.788472	1.290644
H	-1.160360	-3.732050	2.444925
H	0.034427	-4.908717	3.018768
C	0.955453	-2.310132	3.340345
H	0.027120	-1.749840	3.474018
H	1.779922	-1.590707	3.320506
H	1.104088	-2.955053	4.212568
C	0.878947	2.534873	0.010505
C	3.203295	-1.405099	-0.520539
C	4.538320	-1.793716	-0.414894
H	5.067632	-1.647887	0.523222
C	5.202008	-2.355869	-1.496726
H	6.241980	-2.649694	-1.399202
C	4.531047	-2.546732	-2.699241
H	5.044705	-2.991975	-3.545072
C	3.197894	-2.171303	-2.808695
H	2.662583	-2.321483	-3.740640
C	2.535374	-1.601721	-1.727063
H	1.492316	-1.314644	-1.830329
C	3.707613	1.437956	-0.042469
C	3.674720	1.571352	-1.431116
H	2.803231	1.233103	-1.981627
C	4.750783	2.127016	-2.109038
H	4.711271	2.225216	-3.188762
C	5.877356	2.549536	-1.411501
H	6.717774	2.981847	-1.944381
C	5.919801	2.418878	-0.029667
H	6.792288	2.750185	0.523710
C	4.836859	1.871476	0.648133
H	4.868432	1.782147	1.730842
C	0.679389	3.480608	1.225532
H	1.667180	2.958595	-0.620209
H	-0.014243	2.505686	-0.609013
C	-0.081095	4.703510	0.701764
C	-0.108147	2.813701	2.351747
C	2.024514	3.971415	1.773092
H	1.857975	4.725934	2.548818
H	2.607377	3.166825	2.227261
H	2.636690	4.425377	0.987342
H	-0.186362	5.455290	1.489719
H	0.446472	5.171426	-0.136849
H	-1.087239	4.439269	0.361040
H	-0.265295	3.526734	3.167602
H	-1.084899	2.448038	2.029064
H	0.428429	1.953914	2.763482

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5 hov-npnt-anti SCF Done: -2559.79338206 A.U.

Ru	1.411810	-0.236200	0.090798
Cl	1.358792	-0.465378	2.425637
Cl	1.380714	-1.034196	-2.119105
N	-1.355424	-0.882607	0.166490
N	-1.281971	1.282821	-0.101969
C	-0.516593	0.178759	0.032101
C	-2.746113	-0.526089	-0.080021
H	-3.395652	-0.986964	0.665899
C	-2.693018	0.994607	0.168649

C	-3.114682	1.394591	1.567368
C	2.230588	1.379368	-0.069279
H	1.730868	2.333740	-0.230931
C	3.668983	1.479057	0.023489
C	4.345328	2.704157	-0.002403
H	3.765670	3.616399	-0.107819
C	5.724978	2.756854	0.109681
H	6.241350	3.709810	0.091169
C	6.442697	1.573364	0.245857
H	7.523688	1.603717	0.333970
C	5.801319	0.338026	0.269065
H	6.386987	-0.566131	0.370860
C	4.418054	0.296438	0.160003
C	4.280226	-2.134491	0.132592
H	5.099833	-2.117406	0.859362
C	3.246937	-3.137650	0.589293
H	2.435108	-3.208581	-0.139942
H	3.716191	-4.121823	0.671923
H	2.839599	-2.856974	1.562538
C	4.791769	-2.412335	-1.267460
H	5.522031	-1.668285	-1.592667
H	5.271444	-3.394983	-1.292533
H	3.955395	-2.405070	-1.970241
O	3.655251	-0.824761	0.183540
C	-0.885975	-2.258586	0.205841
H	-0.895419	-2.686589	-0.804257
H	0.163731	-2.217759	0.521043
C	-1.585627	-3.231085	1.181910
C	-2.898030	-3.778757	0.609242
H	-3.297564	-4.548725	1.277162
H	-3.672046	-3.017429	0.493682
H	-2.737706	-4.237167	-0.371850
C	-0.621237	-4.414125	1.338888
H	-0.371061	-4.855420	0.367818
H	0.308688	-4.101511	1.823807
H	-1.075951	-5.196659	1.953485
C	-1.811866	-2.590455	2.550653
H	-0.881513	-2.176159	2.947777
H	-2.542709	-1.777955	2.513601
H	-2.187569	-3.340255	3.254572
C	-0.872499	2.671852	-0.171105
C	-3.246616	-0.878550	-1.465395
C	-4.614368	-1.078018	-1.655104
H	-5.286882	-1.034214	-0.801789
C	-5.123955	-1.334603	-2.921117
H	-6.189671	-1.490531	-3.053646
C	-4.266712	-1.401740	-4.013743
H	-4.660987	-1.607736	-5.003382
C	-2.902332	-1.214016	-3.829911
H	-2.224332	-1.273983	-4.674973
C	-2.391180	-0.953149	-2.562882
H	-1.320098	-0.822743	-2.432950
H	-3.330665	1.507756	-0.552120
C	-4.408650	1.871885	1.772451
C	-4.850367	2.199057	3.048780
C	-3.995531	2.057057	4.134864
C	-2.700809	1.590304	3.936372
C	-2.258306	1.260990	2.660900
H	-5.075826	1.992003	0.922601

H	-5.858871	2.572849	3.192862
H	-4.334735	2.315604	5.132555
H	-2.025505	1.480685	4.778492
H	-1.242451	0.900266	2.524020
C	-0.876654	3.324658	-1.572117
H	-1.565301	3.234210	0.467189
H	0.104130	2.770101	0.298338
C	-0.471957	4.786584	-1.366434
C	0.104413	2.645983	-2.527892
C	-2.276240	3.277036	-2.189689
H	-2.293479	3.854525	-3.119356
H	-2.568606	2.253062	-2.440060
H	-3.029344	3.705996	-1.518990
H	-0.438525	5.312383	-2.325236
H	-1.182691	5.312911	-0.719911
H	0.520467	4.865043	-0.909123
H	-0.012128	3.059282	-3.535033
H	1.144044	2.803771	-2.229916
H	-0.059269	1.567210	-2.584791

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6 hov-cychex-syn SCF Done: -2635.95272585 A.U.

Ru	1.585075	0.281264	0.117053
Cl	1.961276	-0.207851	2.370518
Cl	1.439143	1.761101	-1.707602
N	-1.102000	1.313580	0.481065
N	-1.179826	-0.888916	0.462998
C	-0.356764	0.195632	0.375520
C	-2.531700	1.039670	0.436361
H	-3.056164	1.605629	1.211817
C	-2.542530	-0.464567	0.824872
H	-2.632708	-0.508502	1.917924
C	1.756837	-1.273131	-0.805692
H	0.914764	-1.876614	-1.156724
C	3.069735	-1.761715	-1.156056
C	3.278792	-2.998184	-1.778272
H	2.414735	-3.609238	-2.021497
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H	4.711661	-4.397395	-2.555436
C	5.647035	-2.635125	-1.750232
H	6.653530	-2.971072	-1.976717
C	5.473537	-1.396684	-1.138809
H	6.338623	-0.790595	-0.903146
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H	3.451880	2.763939	0.470947
H	5.079379	2.996742	1.128773
H	4.013565	1.757851	1.830824
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H	5.595589	1.135496	-2.132795
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H	-1.751297	-5.167378	2.112510
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C	-1.060846	-2.463130	2.405933
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Ru	-1.439766	-0.299758	-0.130588
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C	-2.172445	1.217378	0.552711
H	-1.629585	1.997689	1.089426
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C	1.500124	-2.700433	-1.651896
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H	2.704288	-5.156493	-1.040314
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H	1.124520	-3.129874	1.769247
H	2.622874	-3.315279	0.856632
C	0.710972	2.545972	0.097342
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C	4.478270	-0.784160	2.172478
H	5.214772	-0.826128	1.373729
C	4.893407	-0.833086	3.497062
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H	1.872558	5.536104	1.125936
H	0.363758	6.401876	0.868216
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H	0.176254	4.737594	2.743705
H	-0.939899	4.384043	1.433743
H	1.761088	3.028019	1.915820
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