Supplementary Information

Base-free synthesis of benchtop stable Ru(III)-NHC complexes from $RuCl_3 \cdot 3H_2O$ and their use as precursors for Ru(II)-NHC complexes

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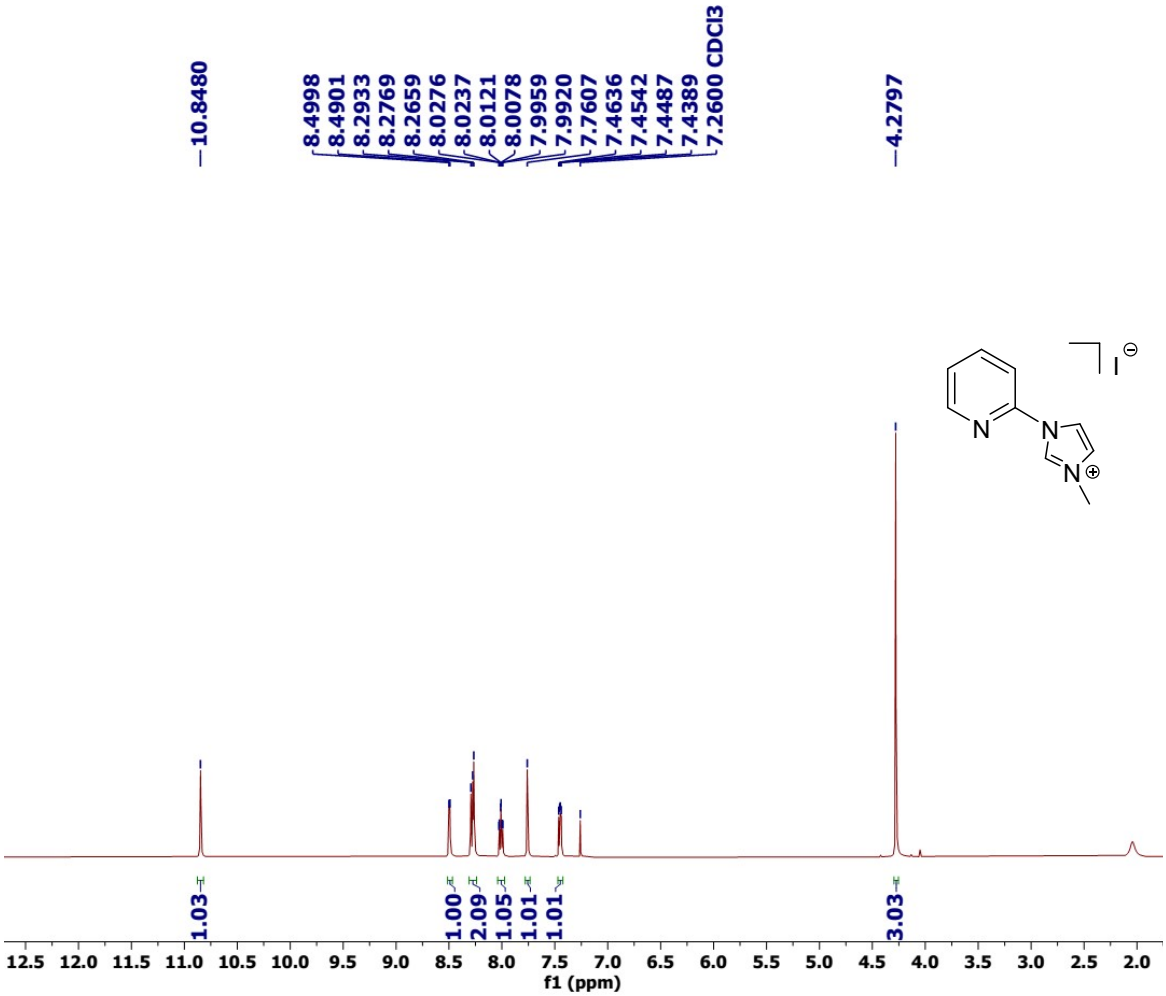

Figure S1. ^{1}H NMR of [3-methyl-1-(pyridin-2-yl)imidazolium]I recorded in $CDCl_3$ at RT.

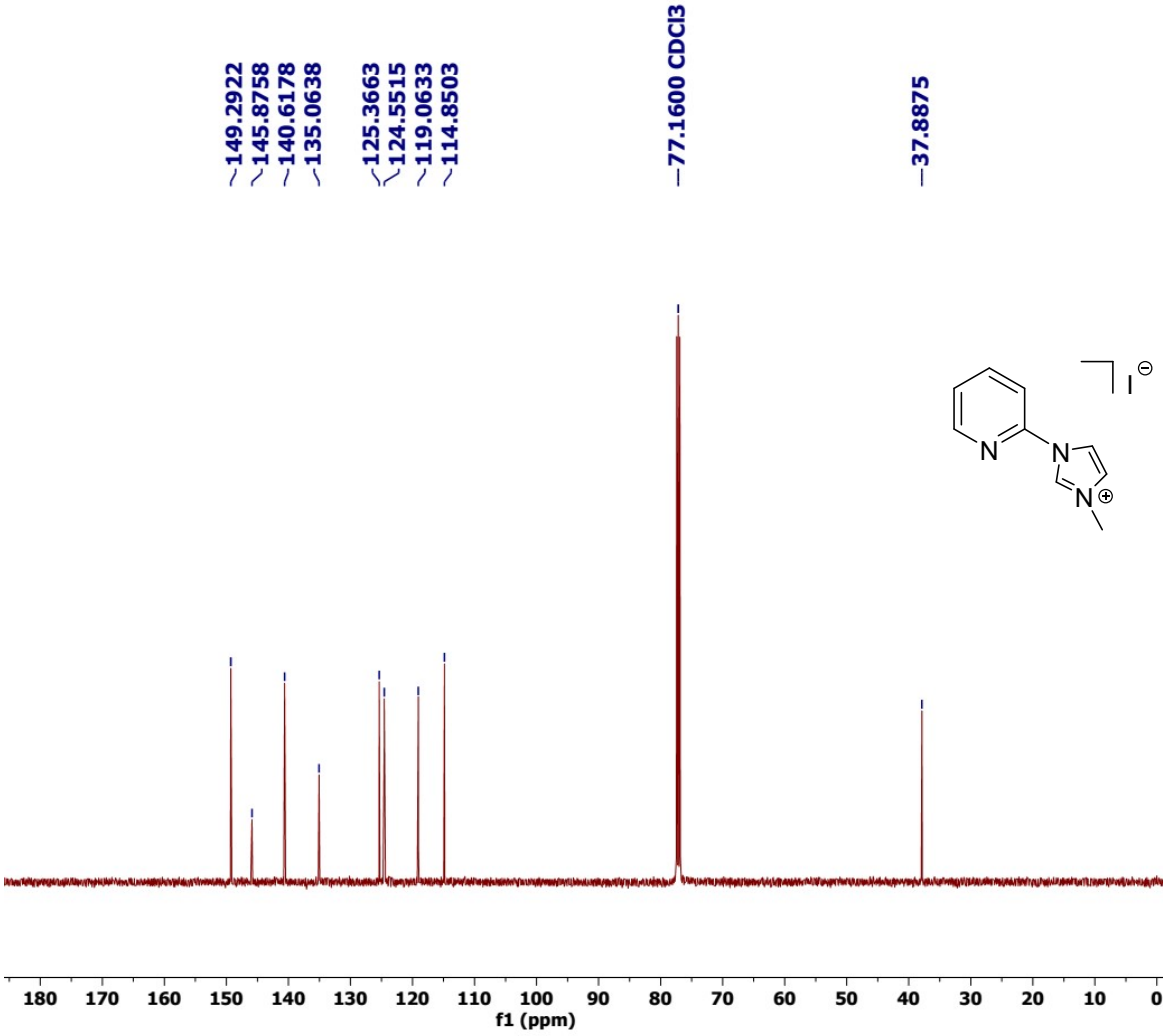

Figure S2. ^{13}C NMR of [3-methyl-1-(pyridin-2-yl)imidazolium]I recorded in $CDCl_3$ at RT.

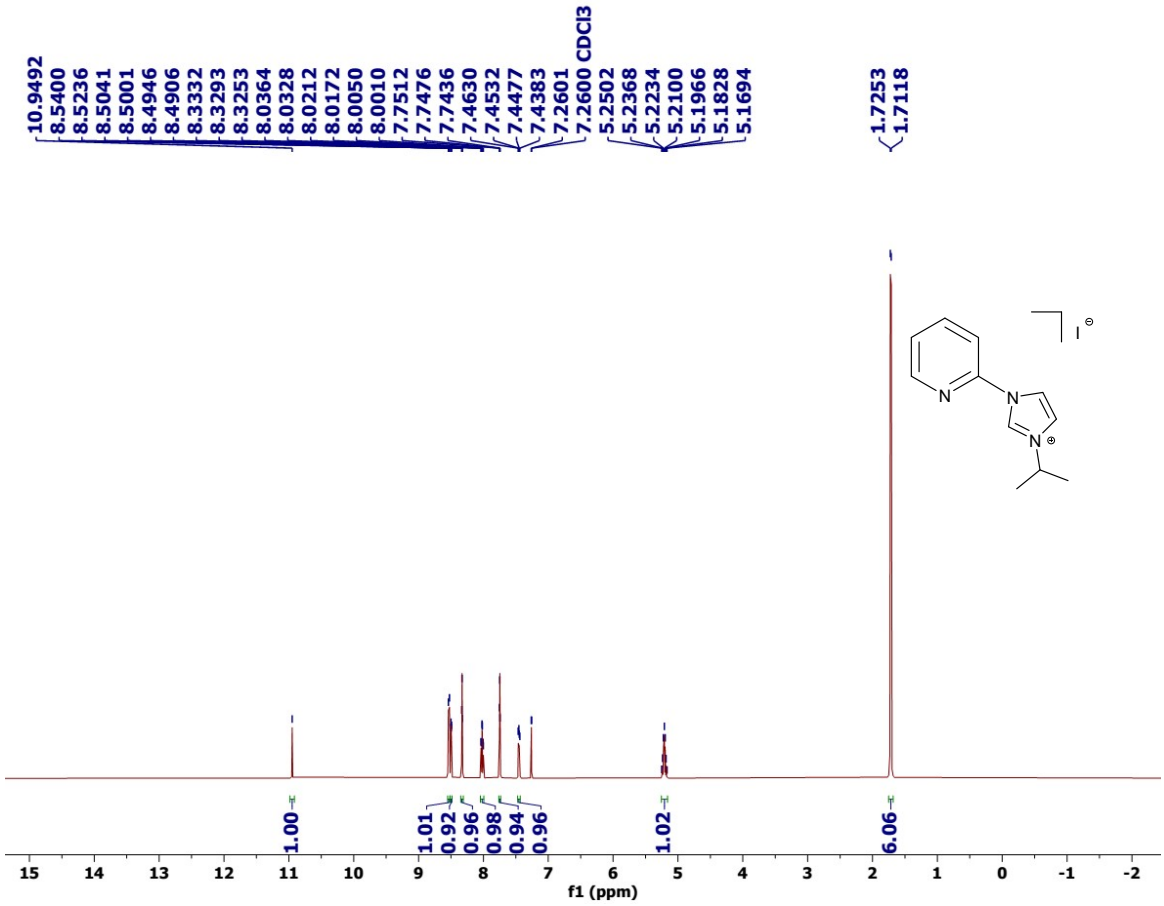

Figure S3. ^{1}H NMR of [3- isopropyl-1-(pyridine-2-yl)imidazolium]Br recorded at a fixed concentration (0.02 mol/L) in $CDCl_3$ at RT.

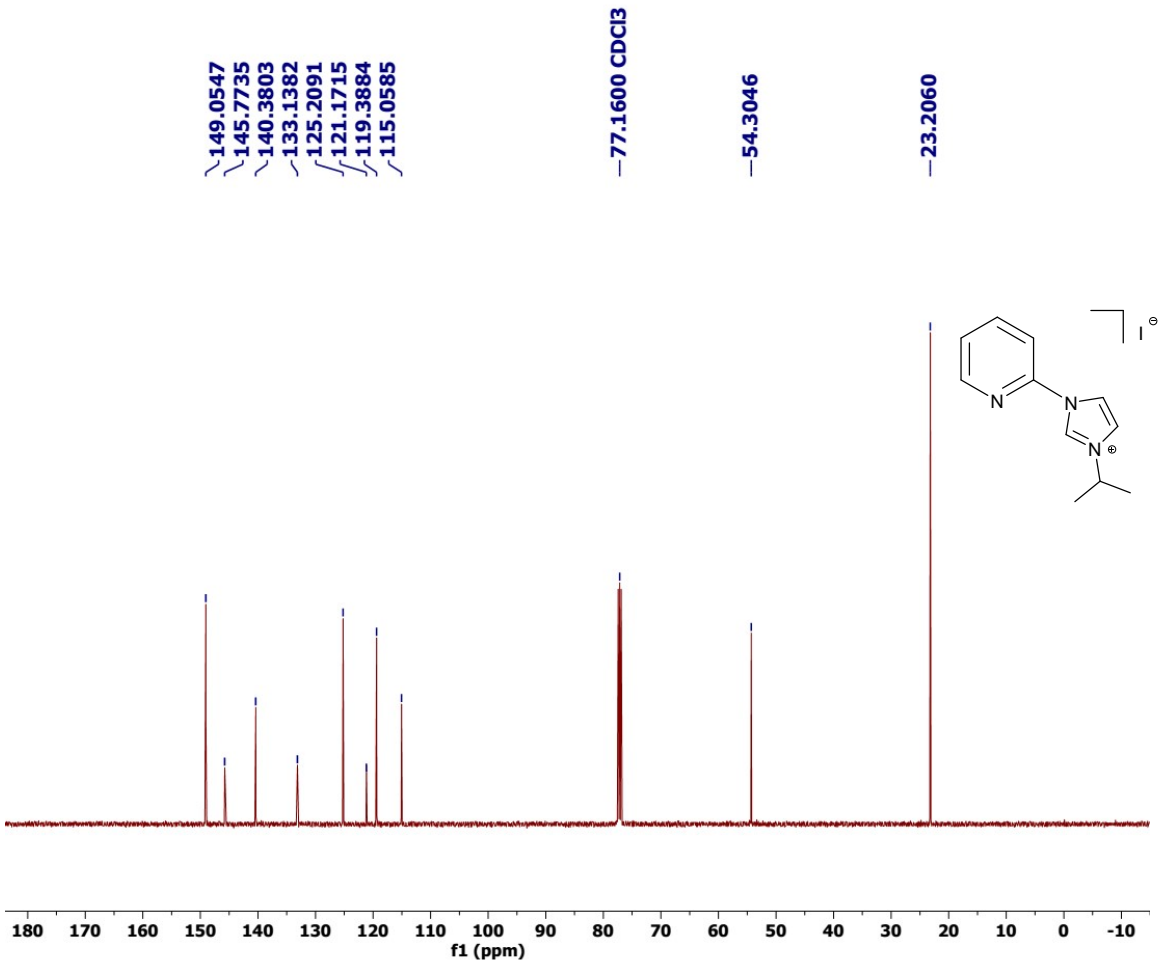

Figure S4. ^{13}C NMR of [3- isopropyl-1-(pyridine-2-yl)imidazolium]Br recorded at a fixed concentration (0.02 mol/L) in $CDCl_3$ at RT.

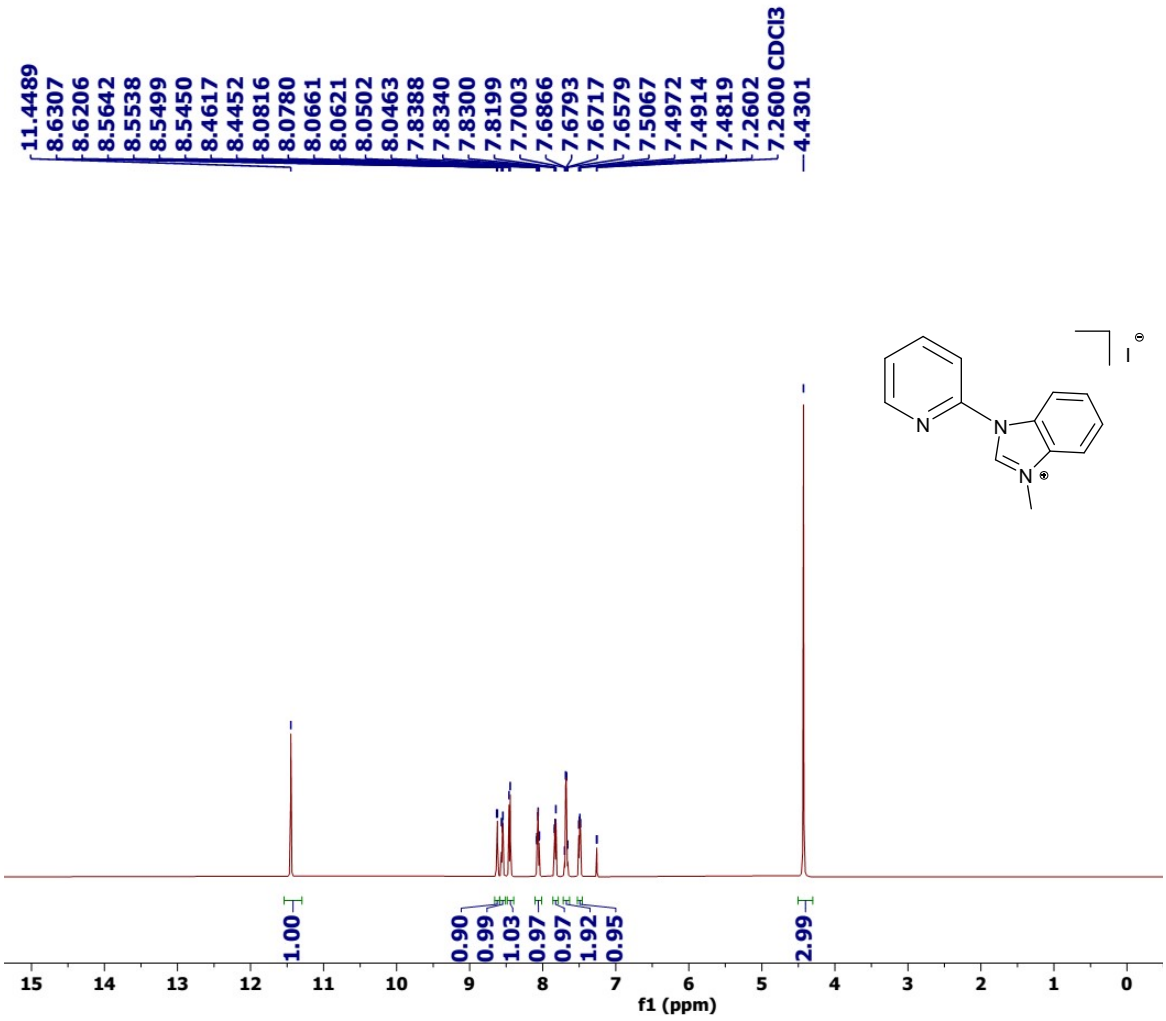

Figure S5. ^{1}H NMR of [3-methyl-1-(pyridin-2-yl)benzimidazolium]I recorded in $CDCl_3$ at RT.

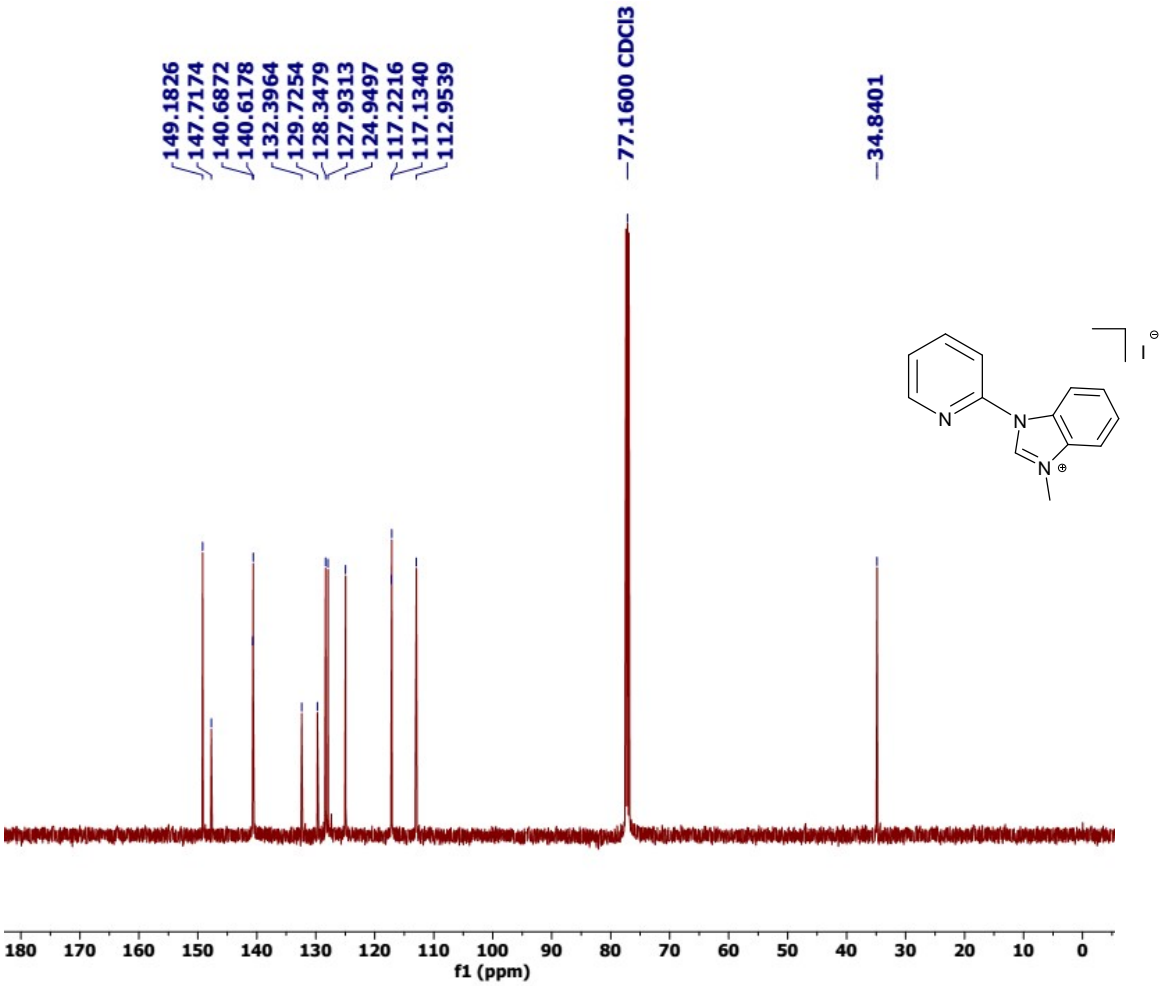

Figure S6. ^{13}C NMR of [3-methyl-1-(pyridin-2-yl)benzimidazolium]I recorded in $CDCl_3$ at RT.

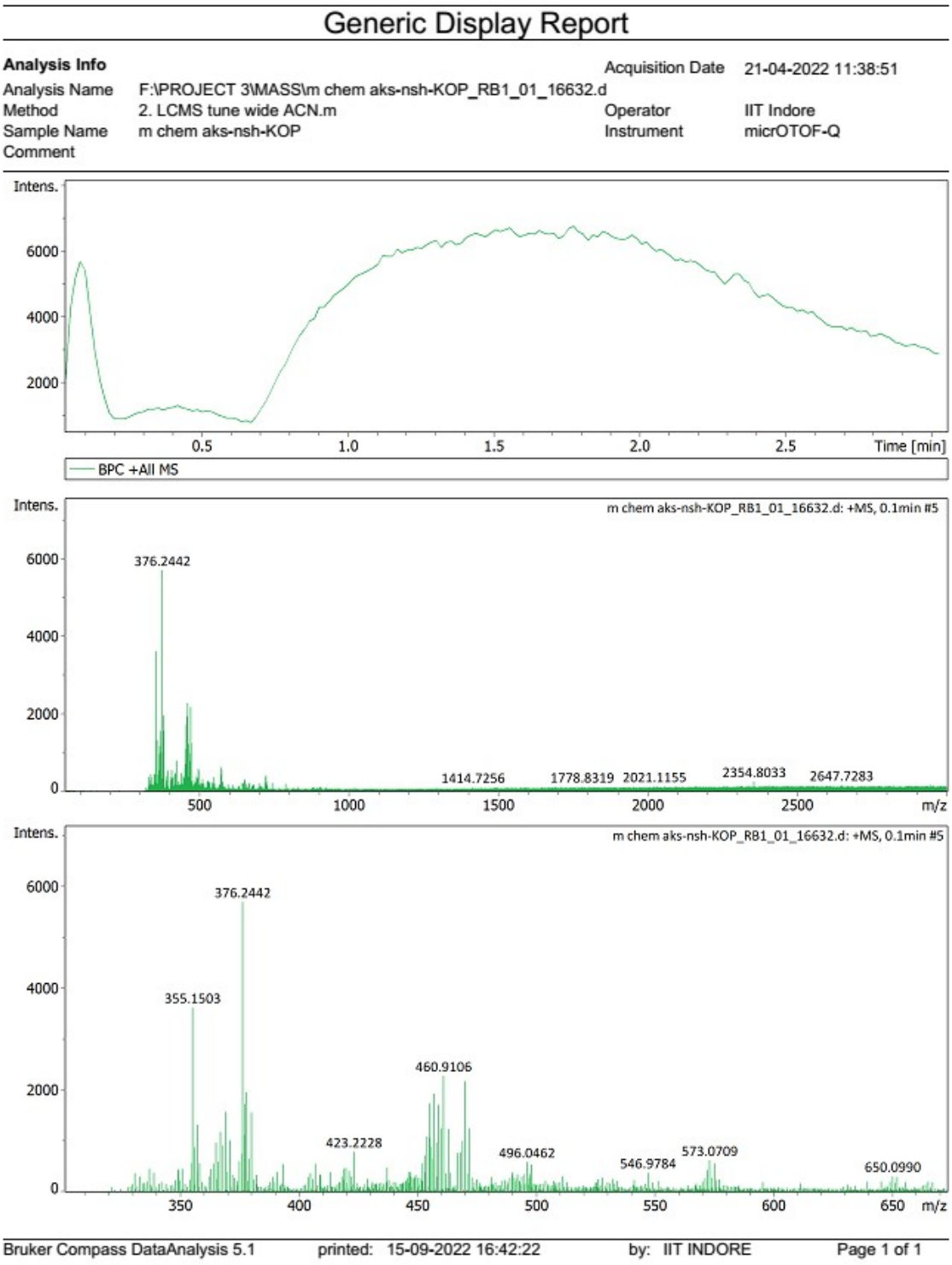

Figure S7. LCMS of attempted synthesis of **1a** in presence of base (KOH) showing no molecular ion peak for the desired parent complex **1a**.

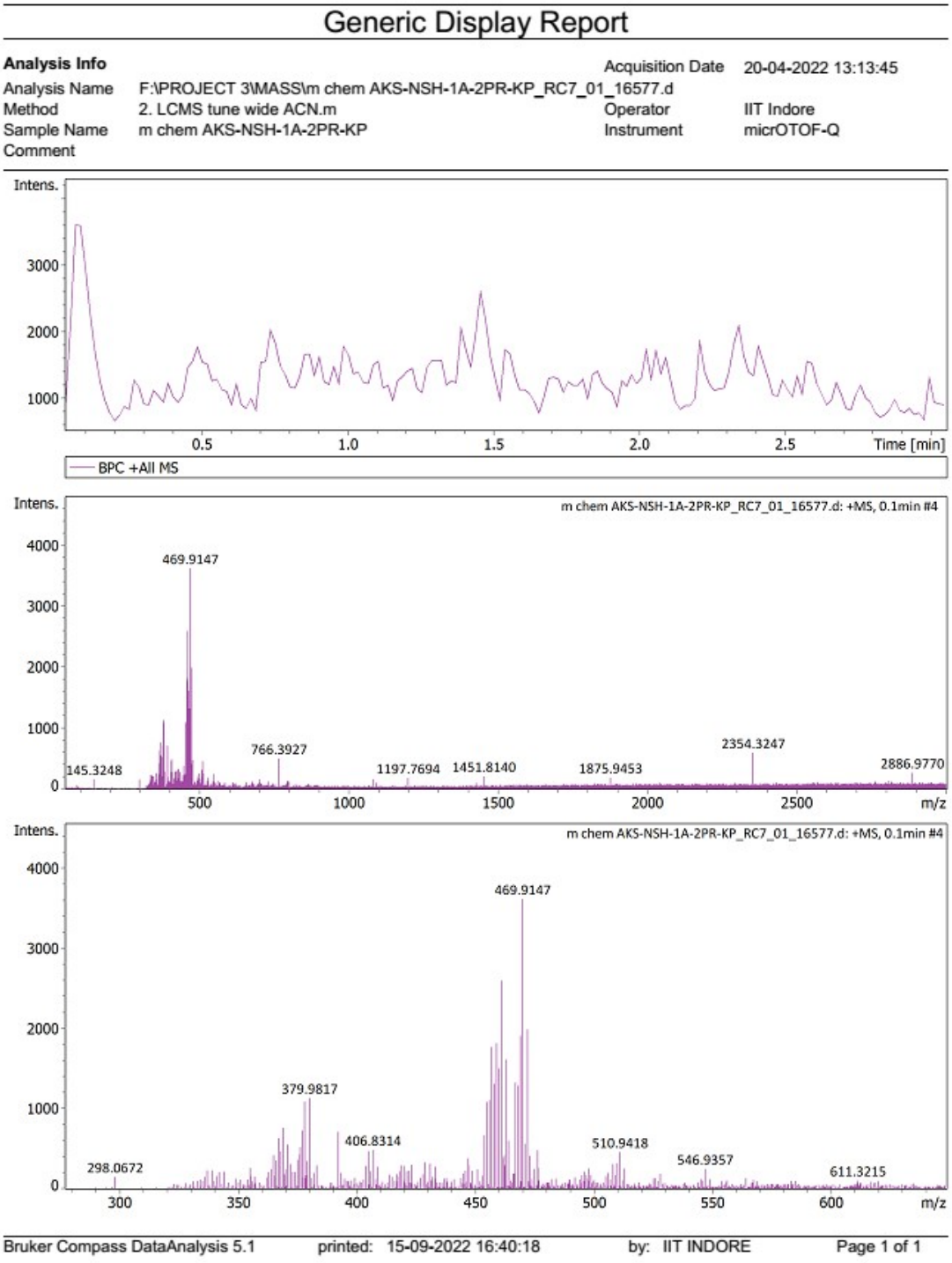

Figure S8. LCMS of attempted synthesis of **1a** in presence of base (K_2CO_3) showing no molecular ion peak for the desired parent complex **1a**.

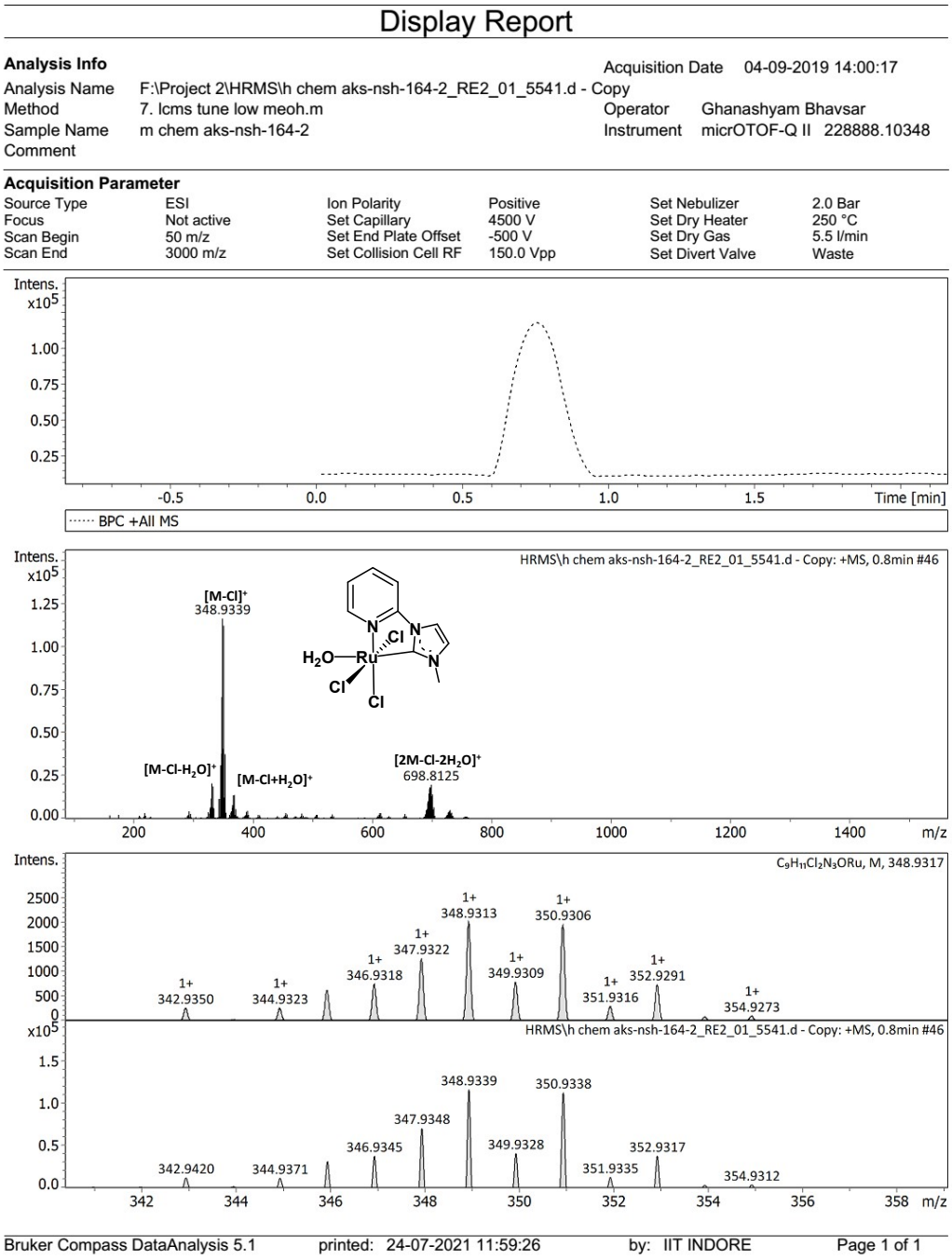

Figure S9. LCMS and HRMS of complex **1a** obtained in absence of base.

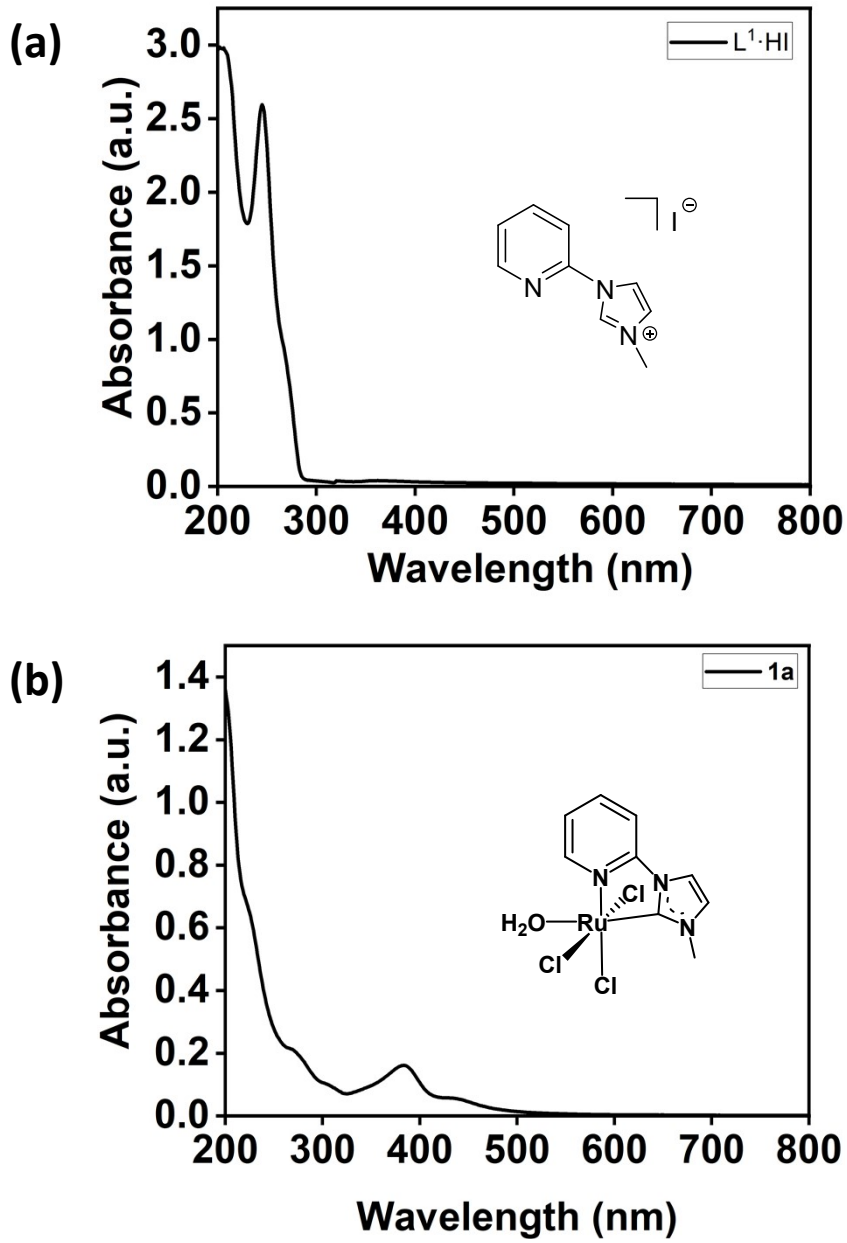

Figure S10. UV-Vis spectra of (a) free ligand L^1·HI and (b) its respective complex **1a** recorded in MeCN

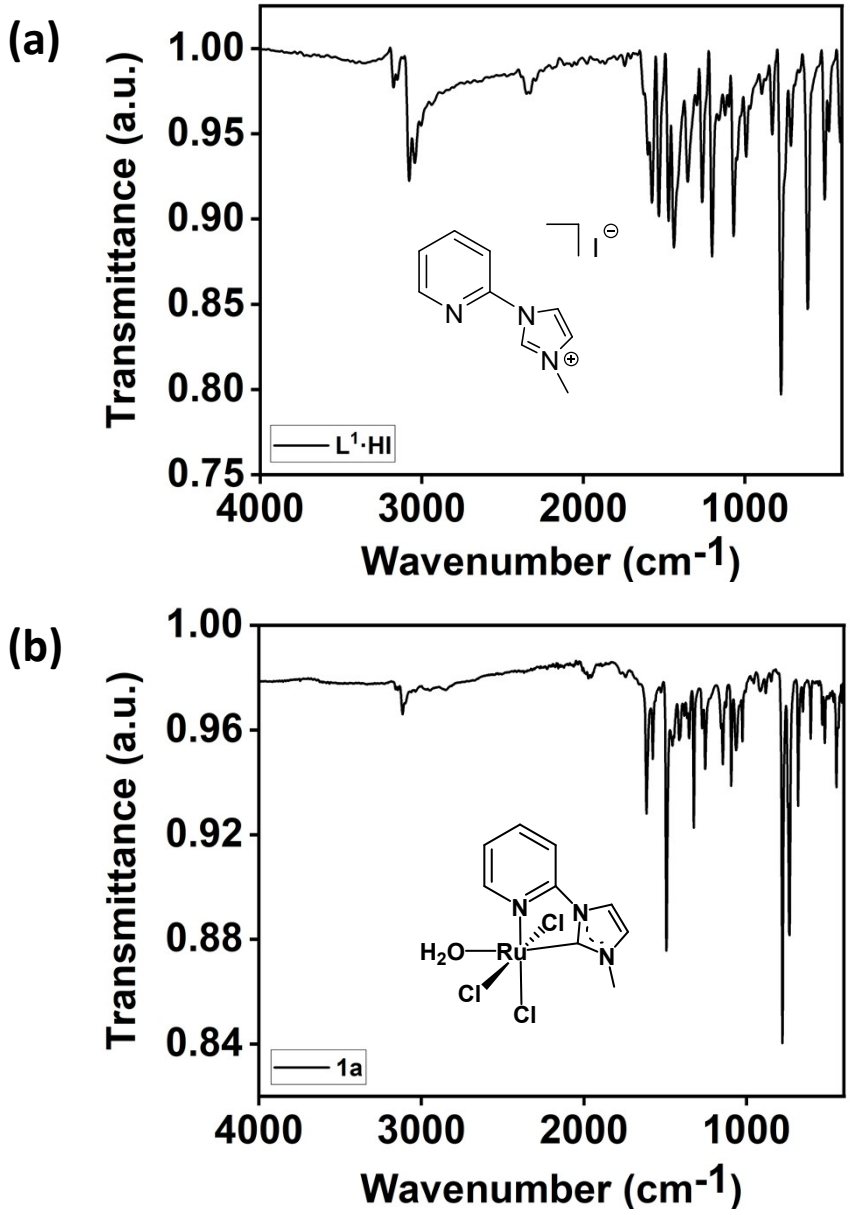

Figure S11. IR spectra of (a) **L[1]·HI** and (b) it's respective complex **1a** in solid state.

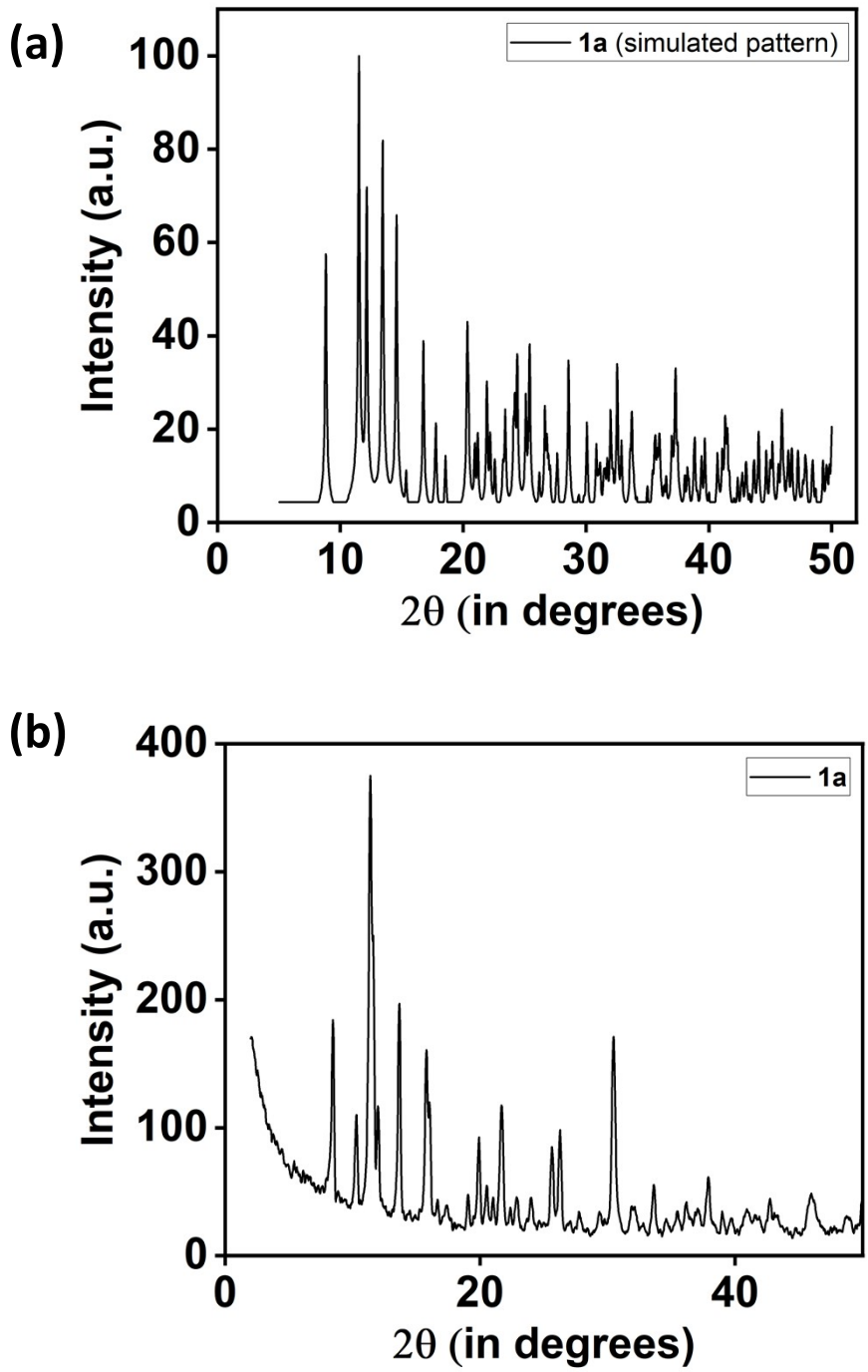

Figure S12. Plots of powder XRD (a) simulated pattern obtained from molecular structure **1a-MeCN** (b) pattern observed experimentally for complex **1a**. Change in position and intensity of signals from the simulated pattern arise due to the existence of solvent molecule (acetonitrile) in the unit cell.

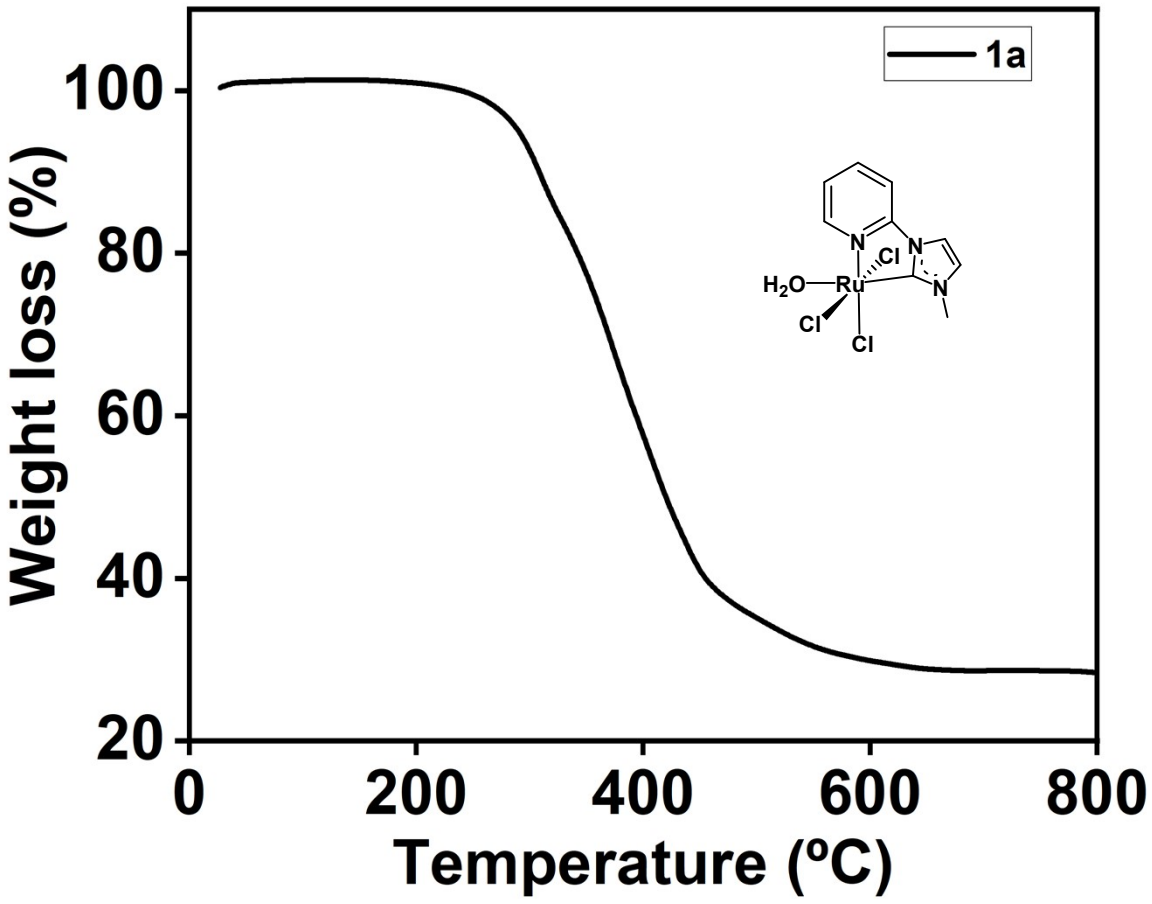

Figure S13. Plot of TGA for complex **1a**. The first derivative curve w.r.t. temperature has revealed that no weight loss was observed up to 300 ºC. Whereas the sequential loss of H_2O molecule and three chlorides was found to occur between 200–450 ºC. Total weight loss was observed to be 71.99% and 28.72% of the compound was remained as residues after complete analysis.

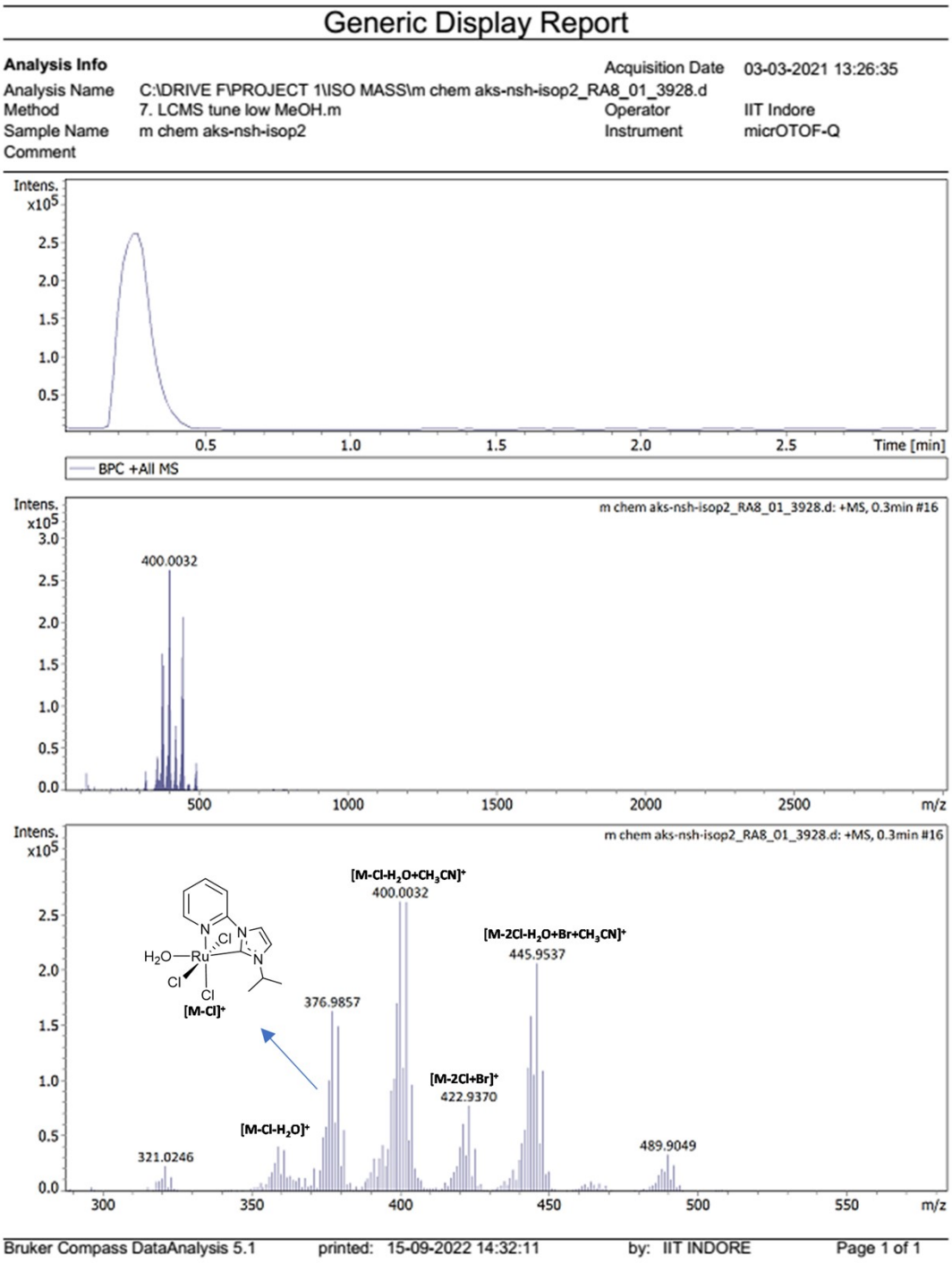

Figure S14. LCMS of complex **1b** synthesized from $L^2 \cdot HBr$ showing the fragments corresponding to $[M\text{-}Cl]^+$ and $[M\text{-}2Cl+Br]^+$ present in the crude sample.

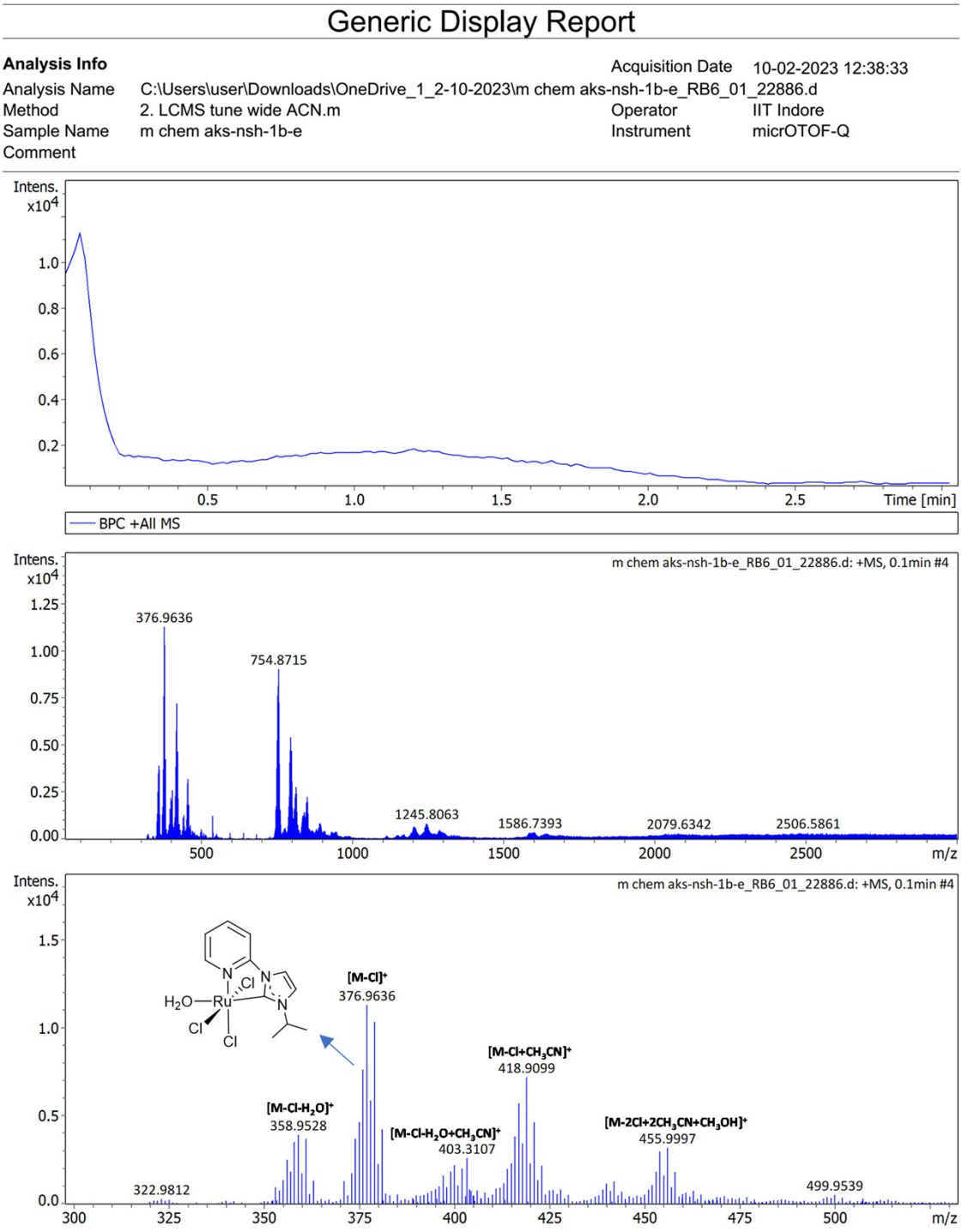

Figure S15. LCMS of complex **1b** synthesized from $L^2 \cdot HI$ showing the fragments corresponding to $[M\text{-}Cl]^+$ and $[M\text{-}2Cl+CH_3CN]^+$ present in the crude sample.

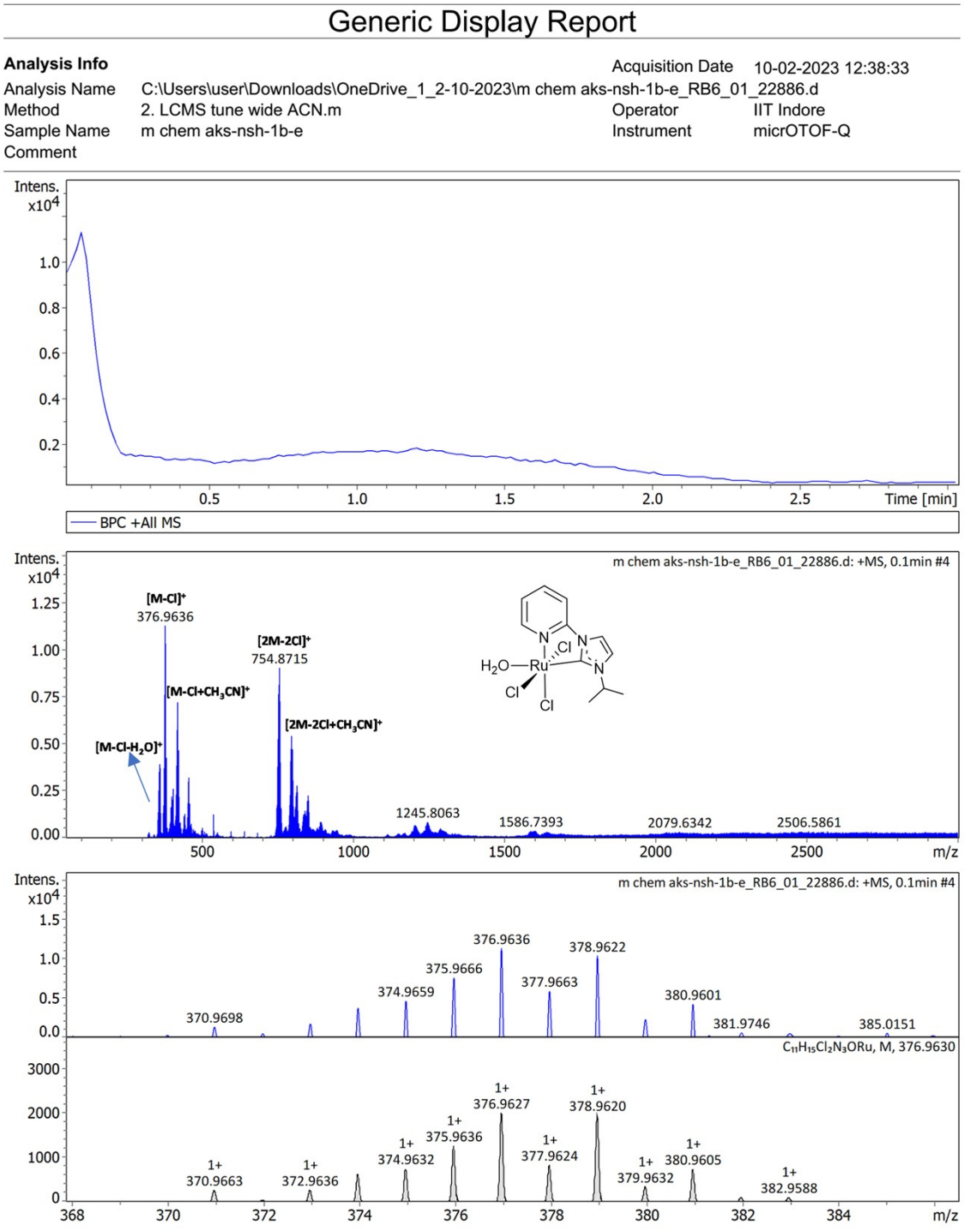

Figure S16. LCMS and HRMS of complex **1b** synthesized from L^2·HI in absence of base.

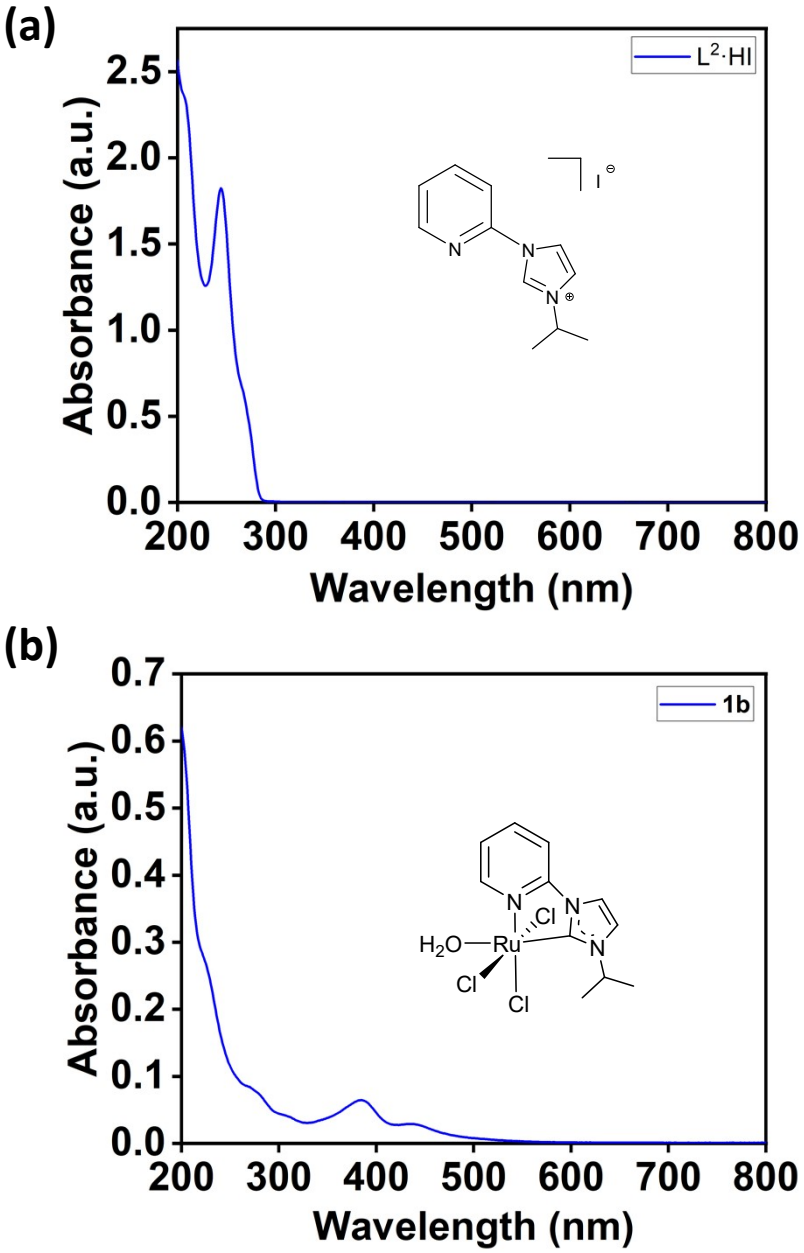

Figure S17. UV-vis spectra of (a) free ligand **L²·HI** and (b) its respective complex **1b** recorded in MeCN at room temperature.

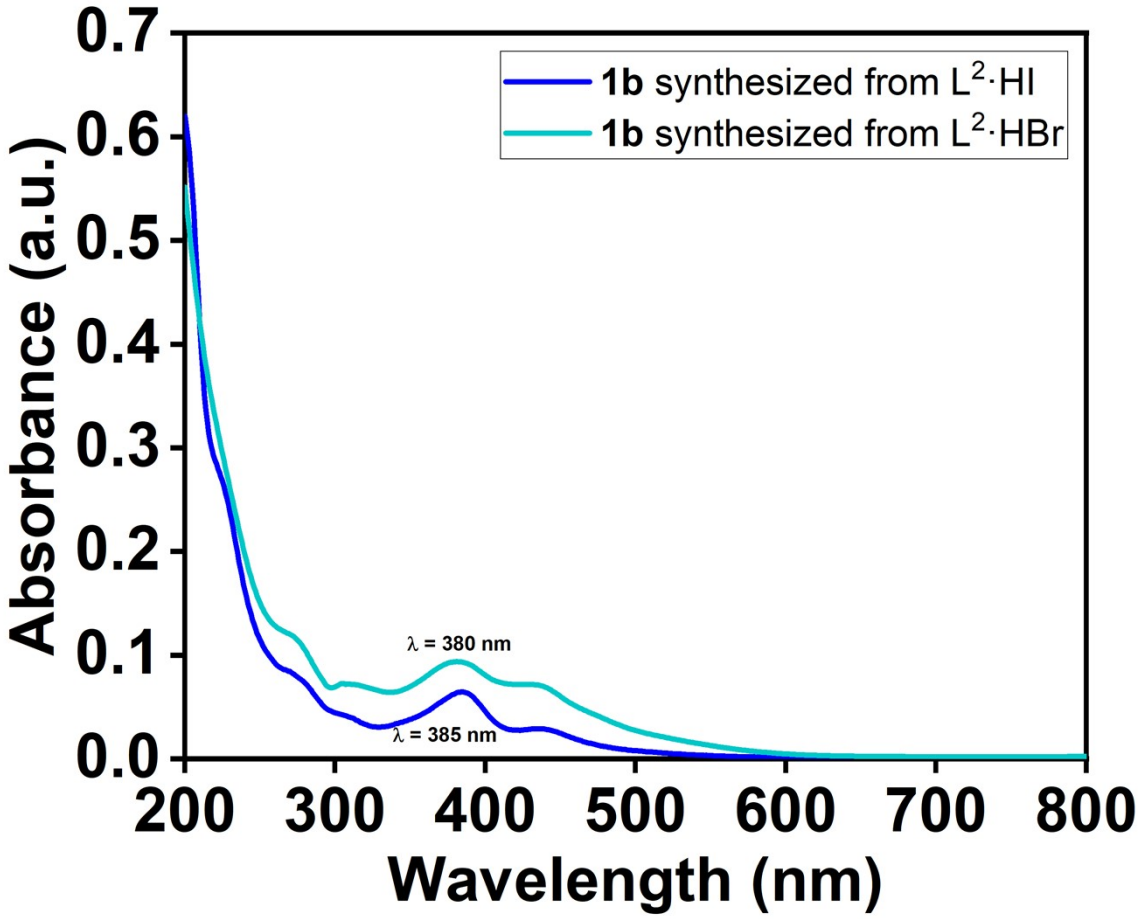

Figure S18. UV-Vis spectra of complex **Ib**, synthesized from **L^2·HI** and **L^2·HBr** respectively, recorded in MeCN at room temperature

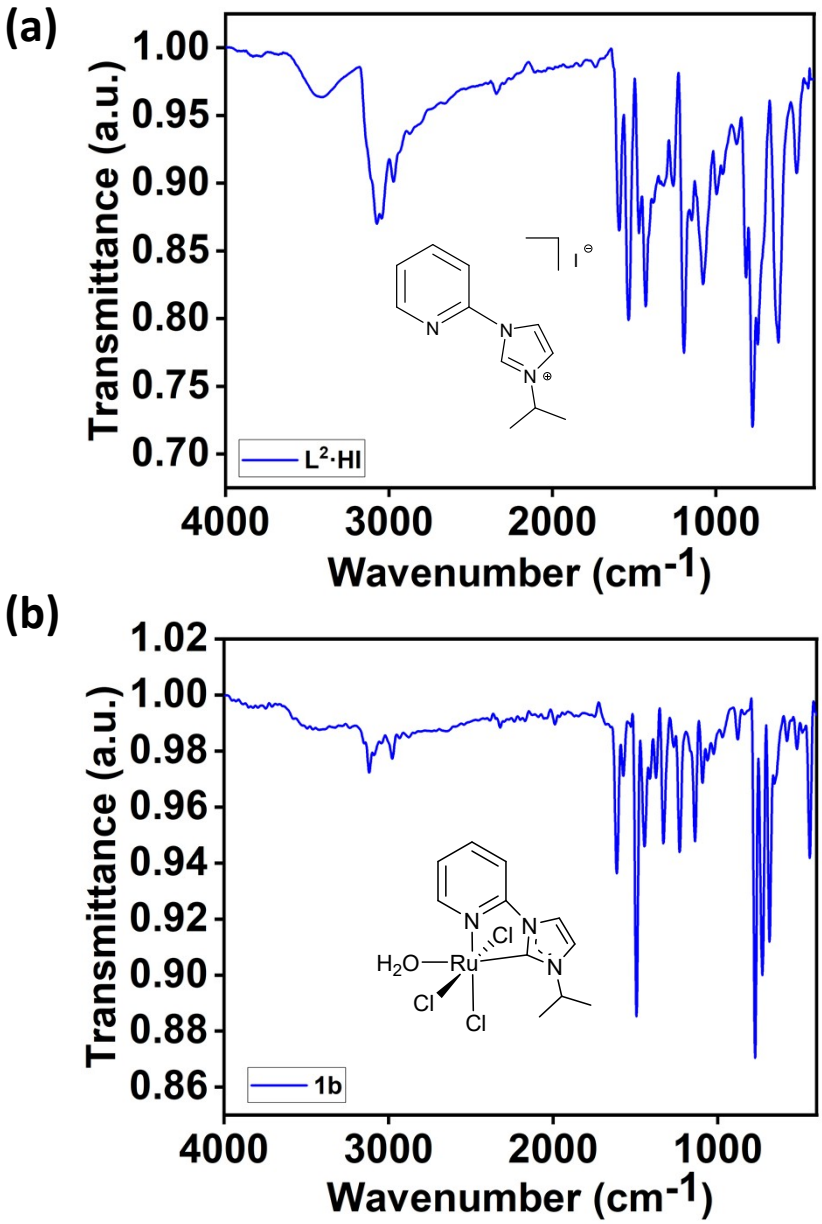

Figure S19. IR spectra of (a) **L²·HI** and (b) it's respective complex **1b** in solid state.

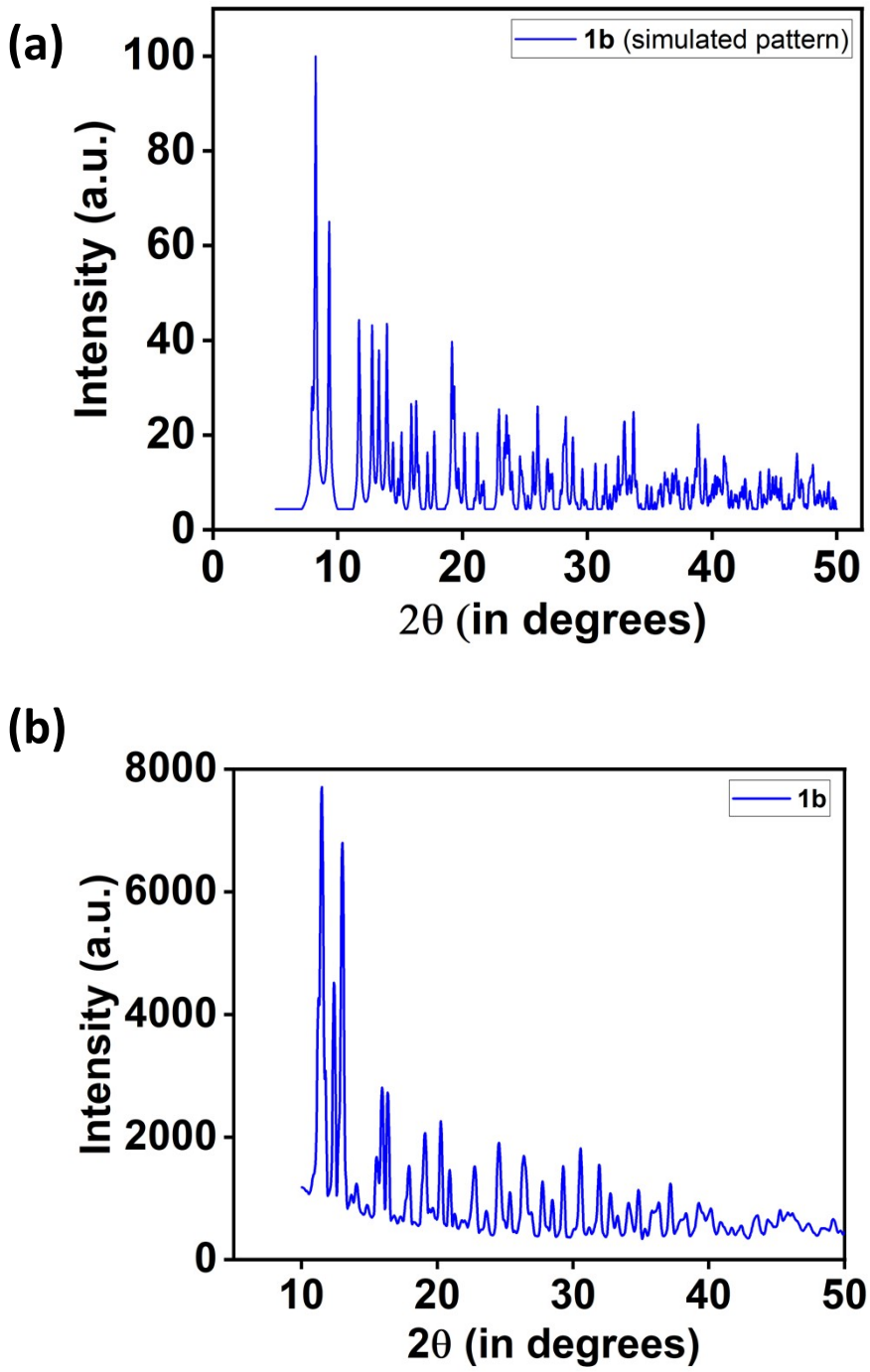

Figure S20. Plots of powder XRD (a) simulated pattern obtained from molecular structure **1b-MeOH** (b) pattern observed experimentally for complex **1b**. Change in position and intensity of signals from the simulated pattern arise due to the existence of solvent molecule (methanol) in the unit cell.

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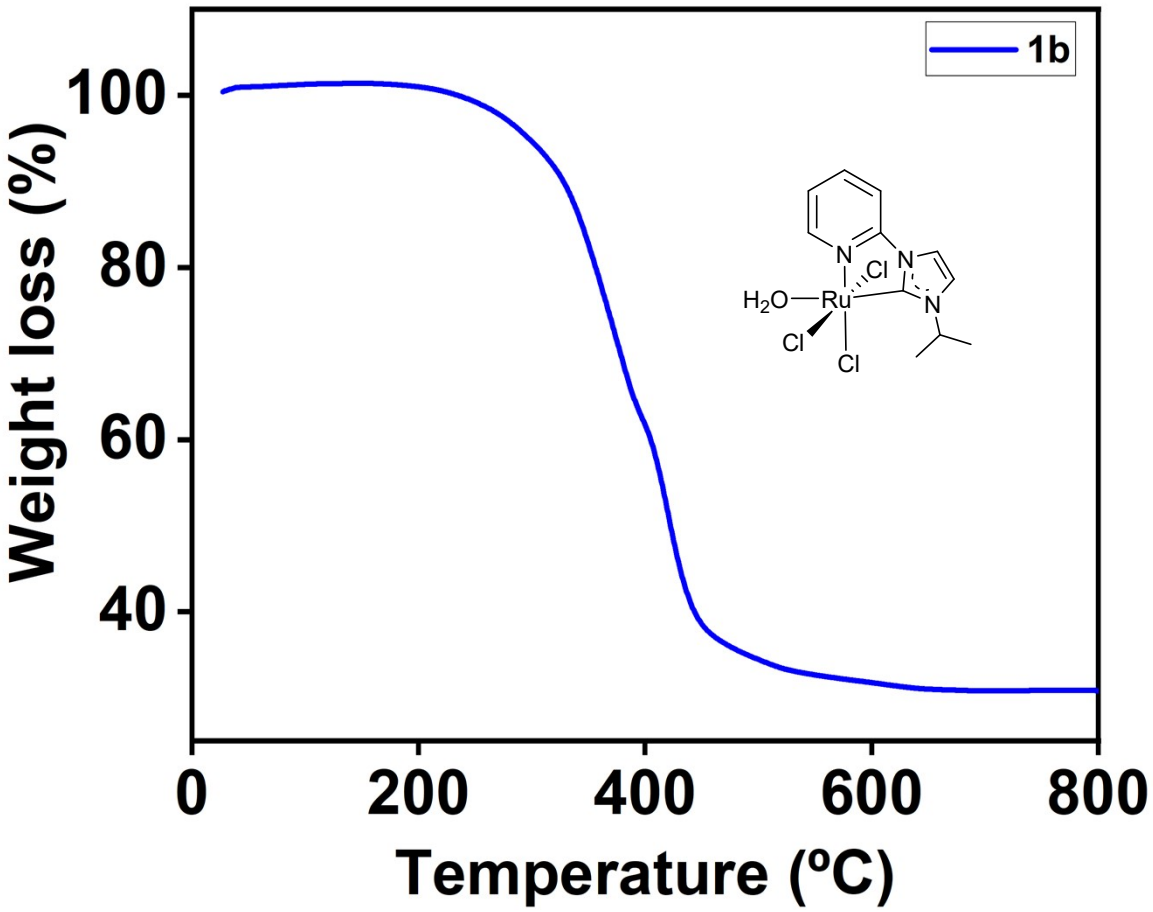

Figure S21. Plot of TGA for complex **1b**. The first derivative curve w.r.t. temperature has revealed that no weight loss was observed up to 230 ºC. Whereas the sequential loss of H_2O molecule and three chlorides was found to occur between 200–420 ºC. Total weight loss was observed to be 69.9% and 31.02% of the compound was remained as residues after complete analysis.

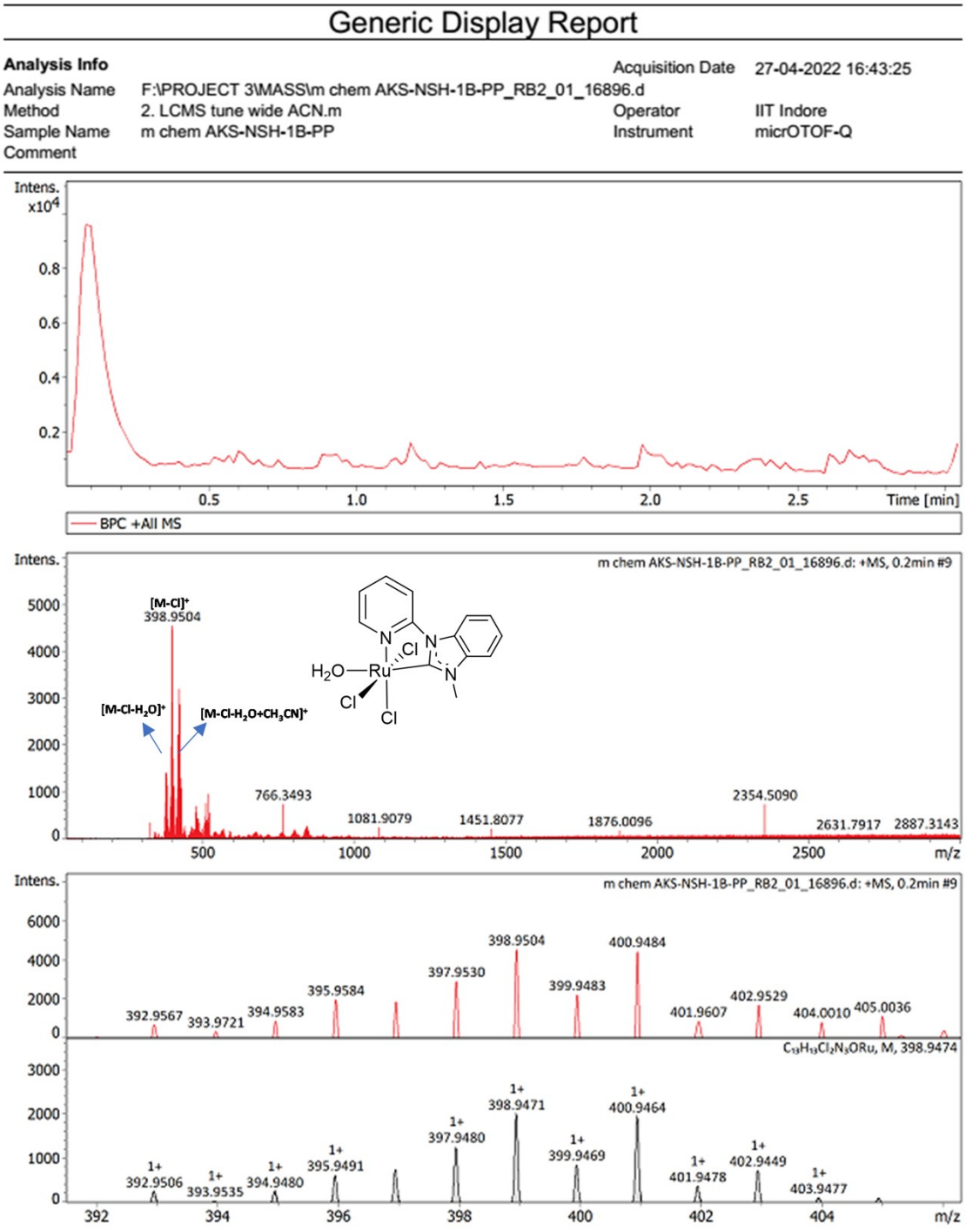

Figure S22. LCMS and HRMS of complex **1c** obtained in absence of base.

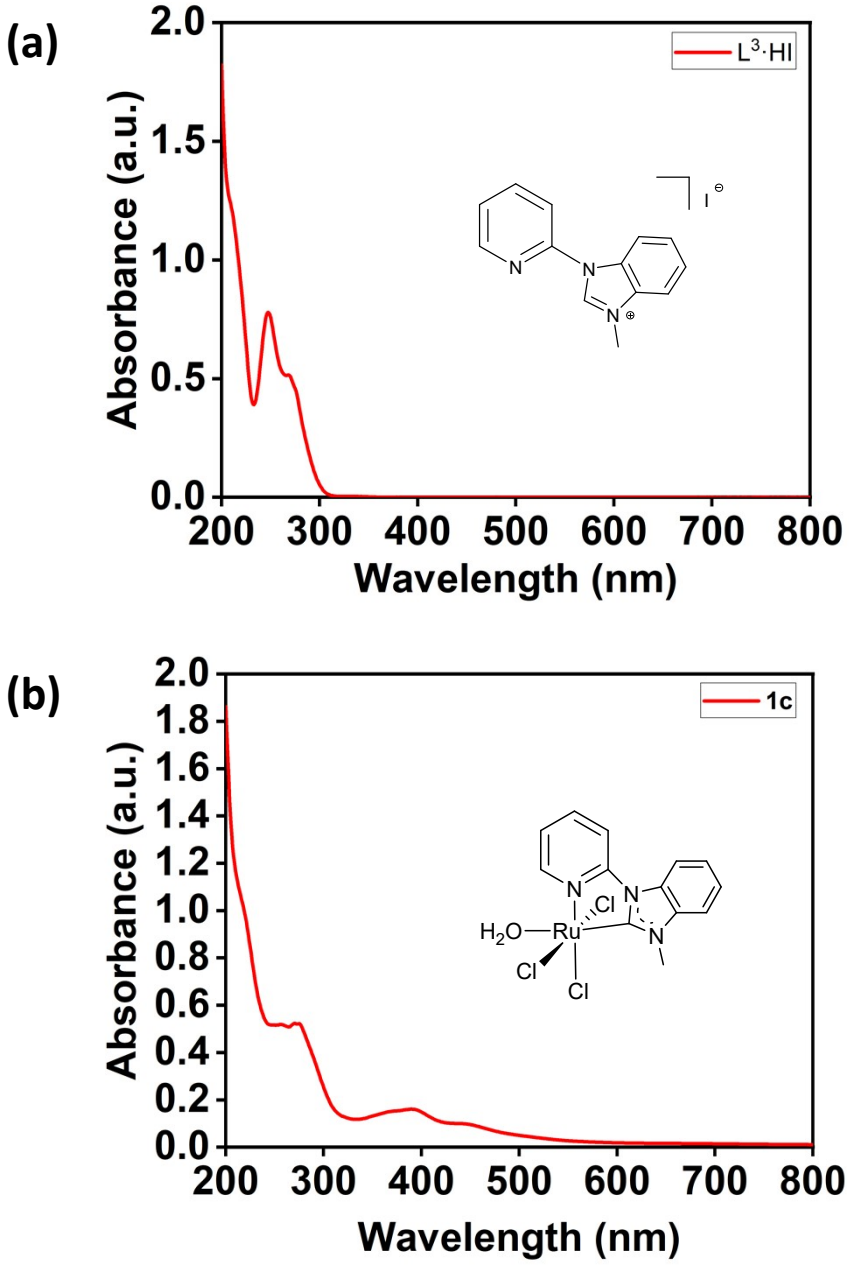

Figure S23. UV-Vis spectra of (a) free ligand **L³·HI** and (b) its respective complex **1c** recorded in MeCN at room temperature.

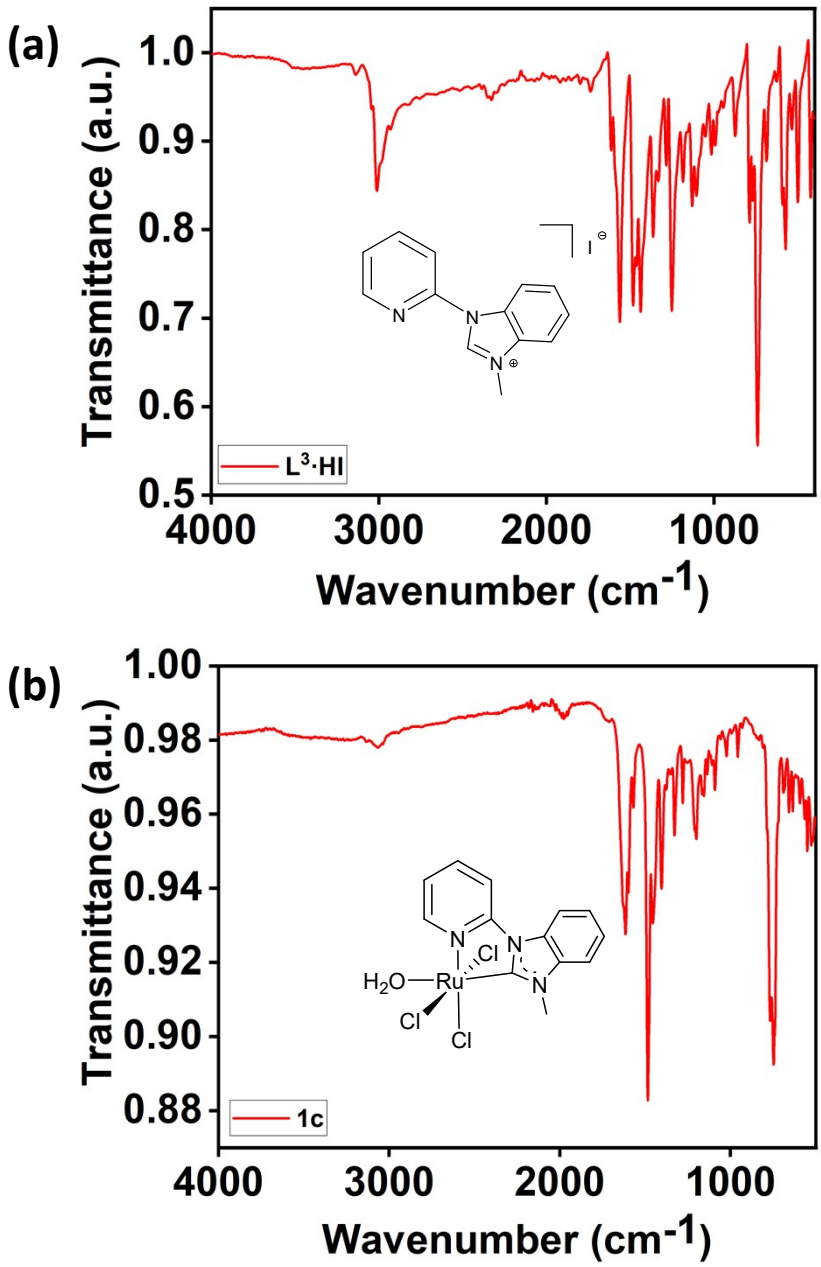

Figure S24. IR spectra of (a) **L³·HI** and (b) it's respective complex **1c** in solid state.

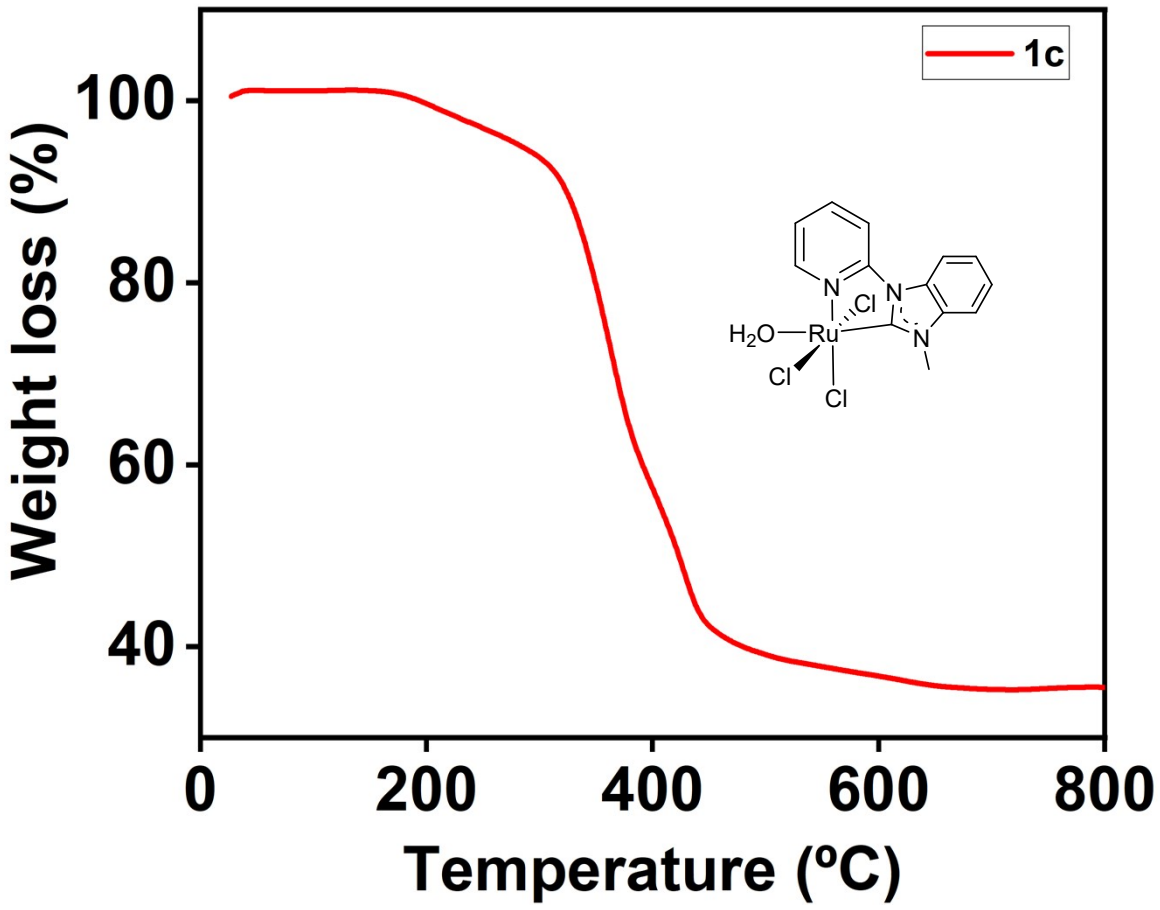

Figure S25. Plot of TGA for complex **1c**. The first derivative curve w.r.t. temperature has revealed that no weight loss was observed up to 150 ºC. Whereas the sequential loss of H_2O molecule and three chlorides was found to occur between 200–420 ºC. Total weight loss was observed to be 65.42 % and 35.42% of the compound was remained as residues after complete analysis.

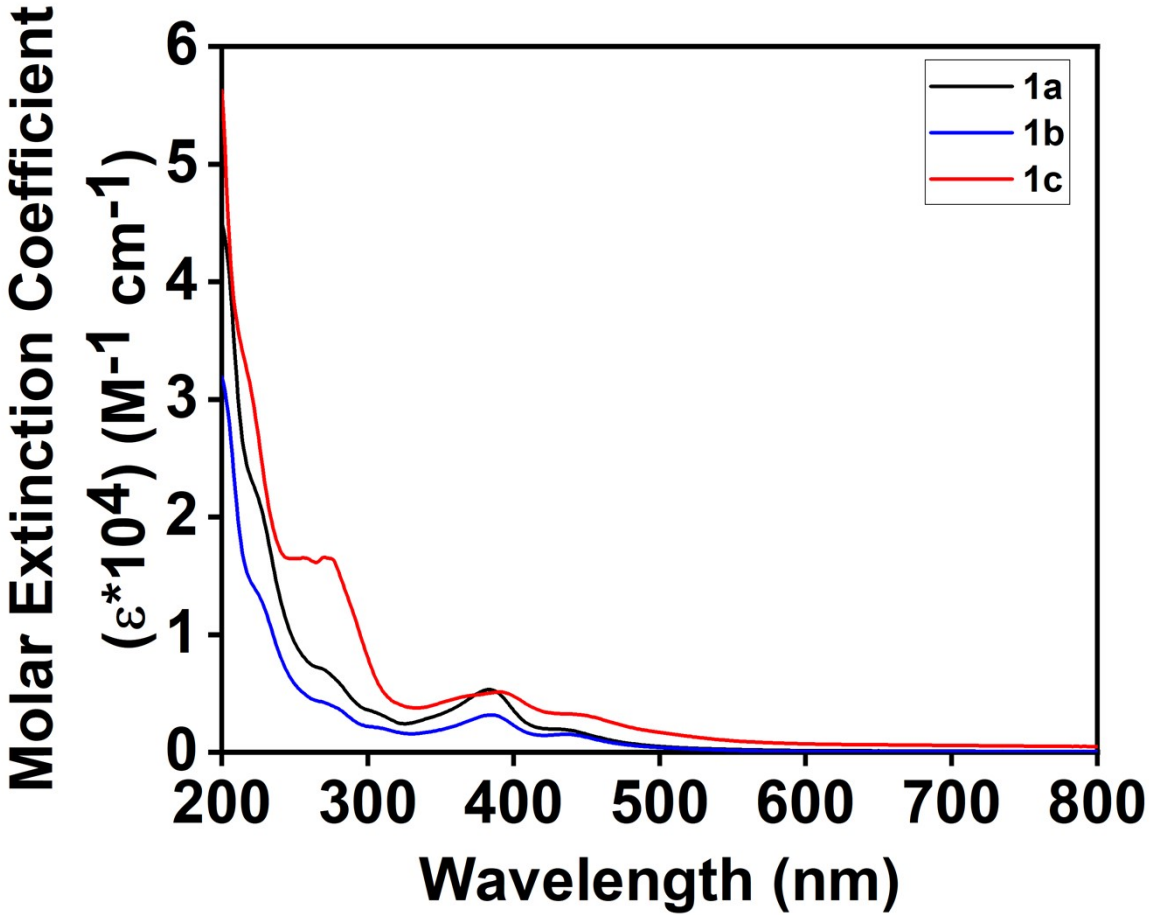

Figure S26. Molar extinction coefficients of complexes **1a–c** recorded in MeCN at room temperature.

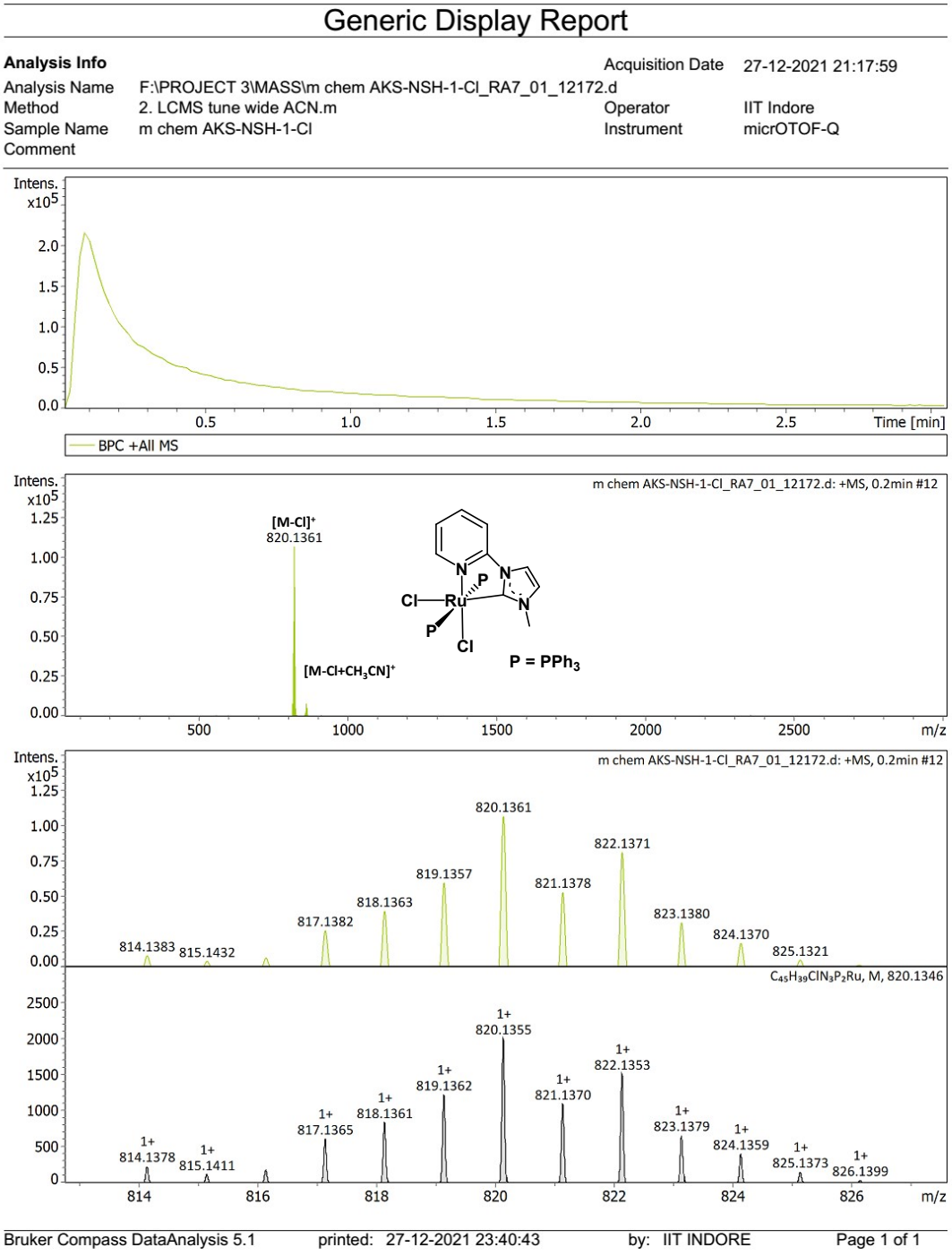

Figure S27. LCMS and HRMS of complex **2a**.

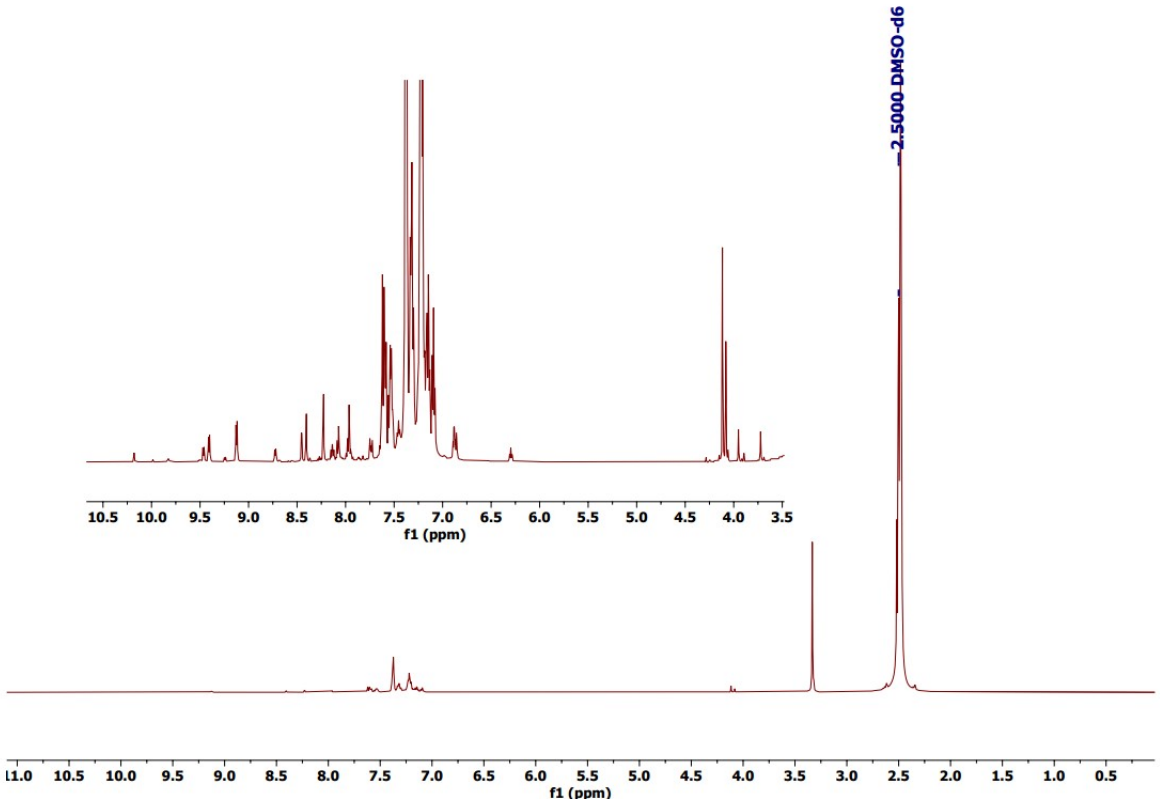

Figure S28. ^{1}H NMR spectrum of **2a** in DMSO-d_6 Peak assignment is difficult due to poor solubility and existence of two species in solution.

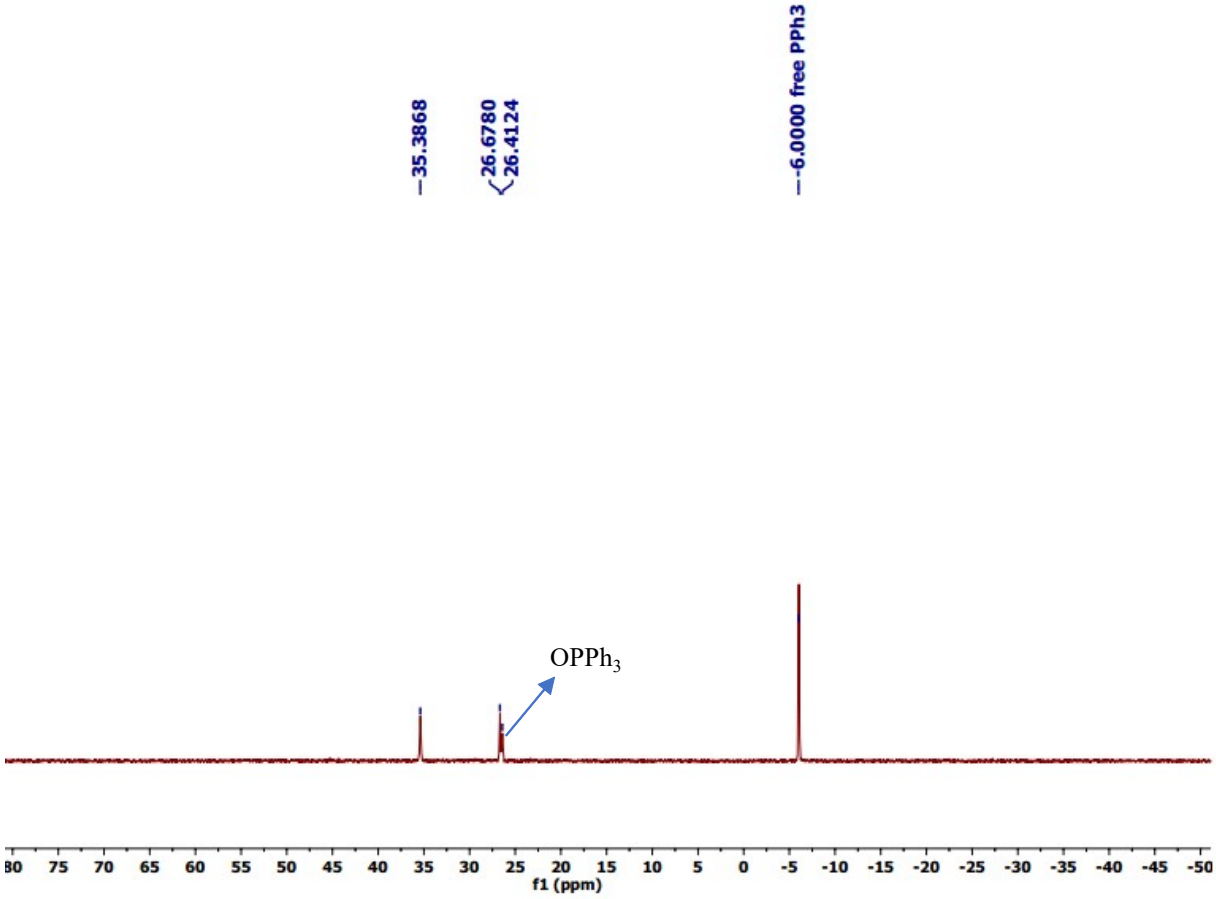

Figure S29. ^{31}P NMR spectrum of complex **2a** in DMSO-d_6. $OPPh_3$ was observed in the spectrum due to the arial oxidation.

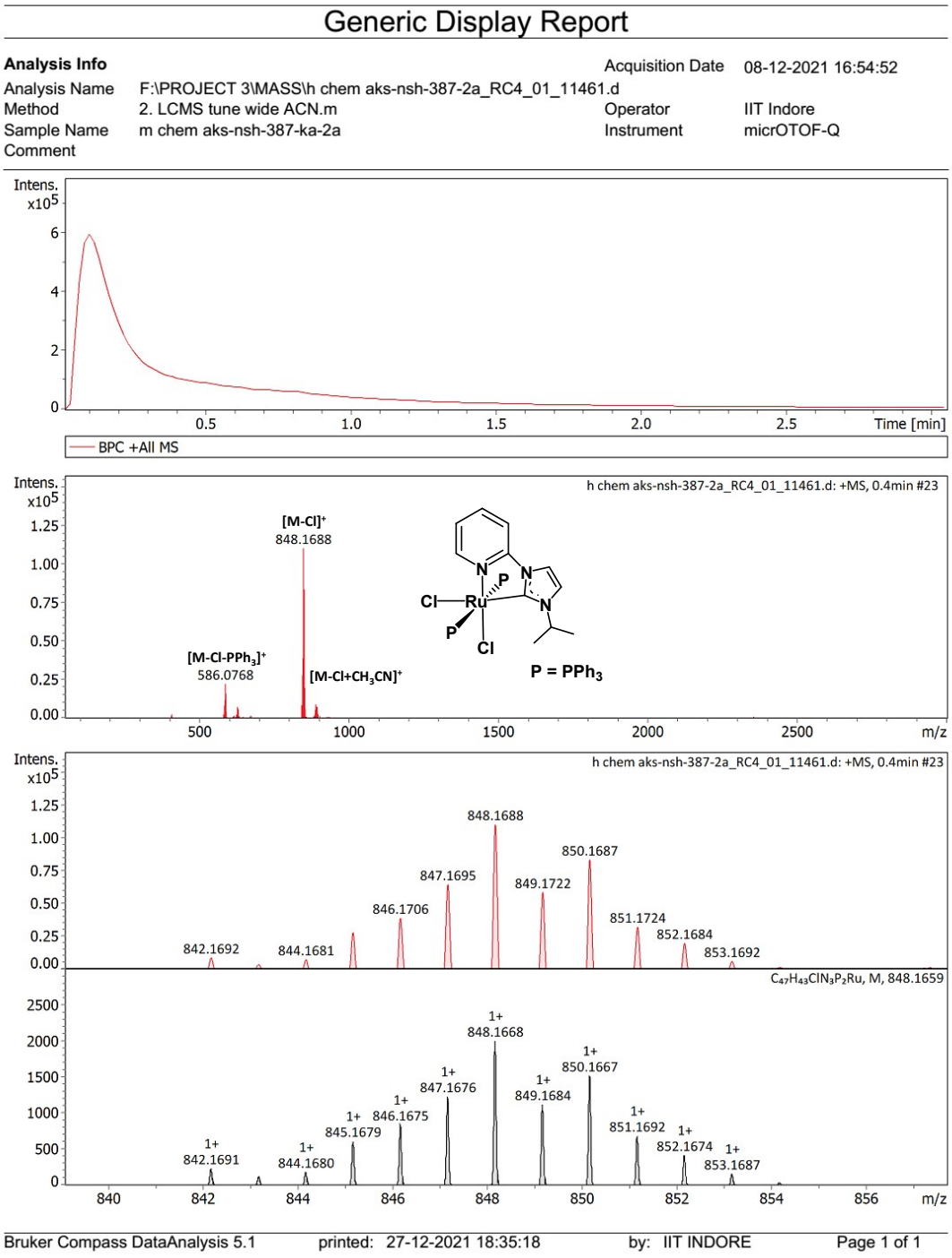

Figure S30. LCMS and HRMS of complex **2b.**

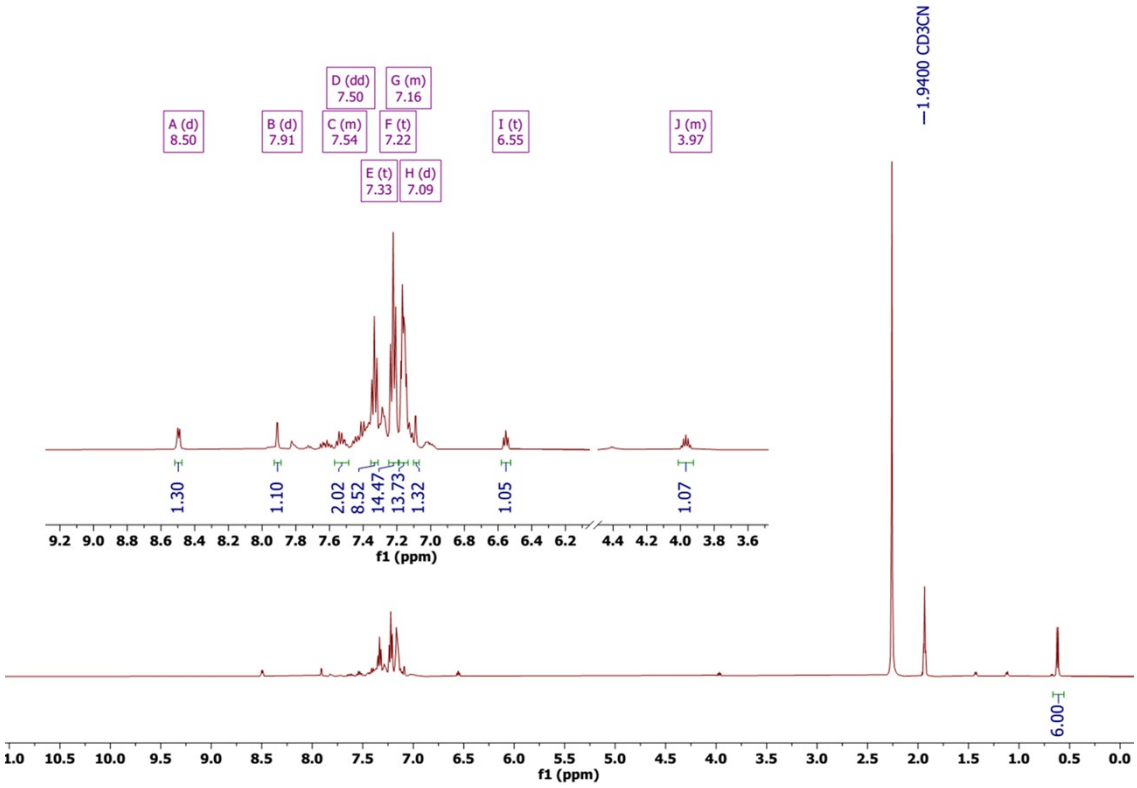

Figure S31. ^{1}H NMR of complex **2b** in CD_3CN.

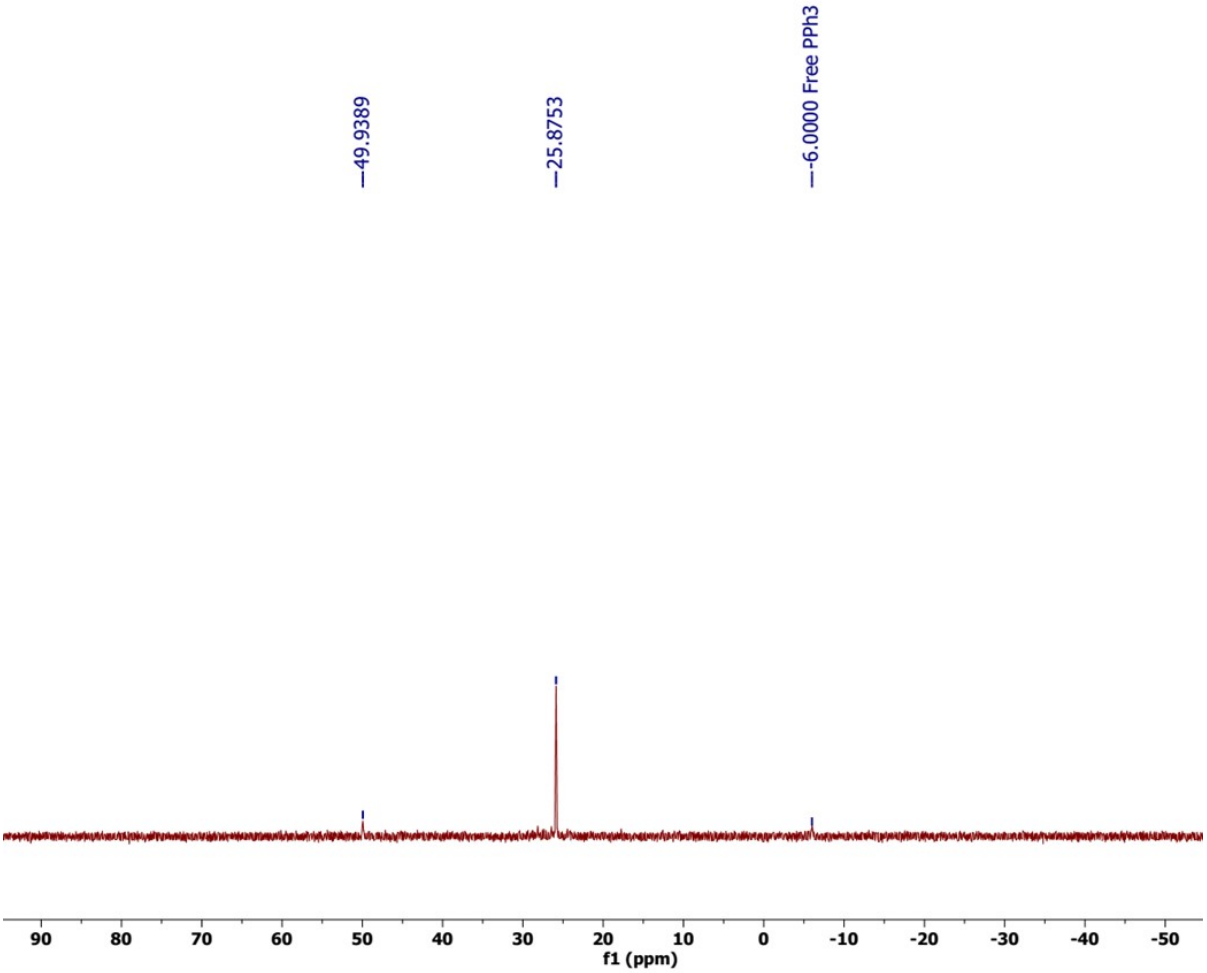

Figure S32. ^{31}P NMR of complex **2b** in CD_3CN.

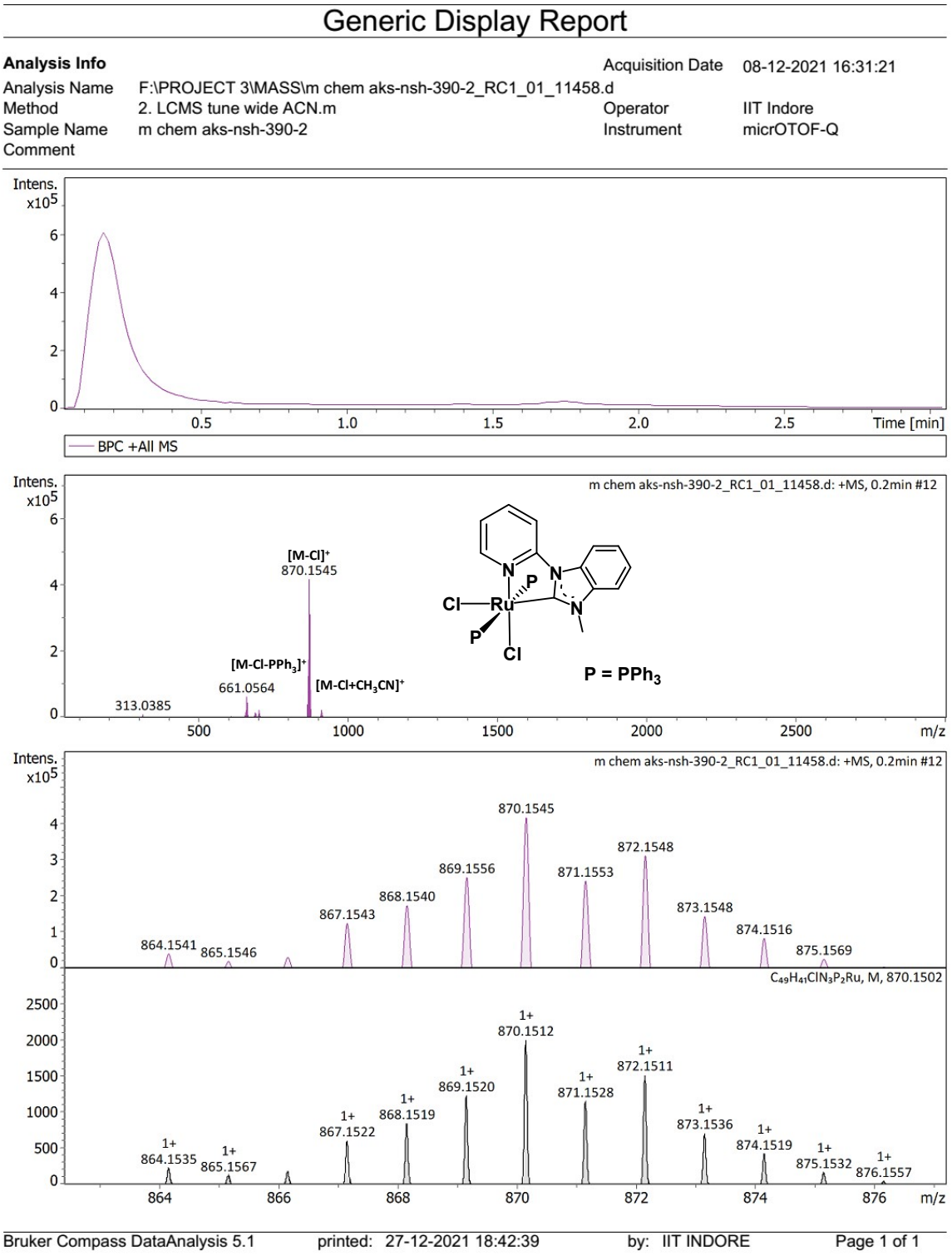

Figure S33. LCMS and HRMS of complex **2c.**

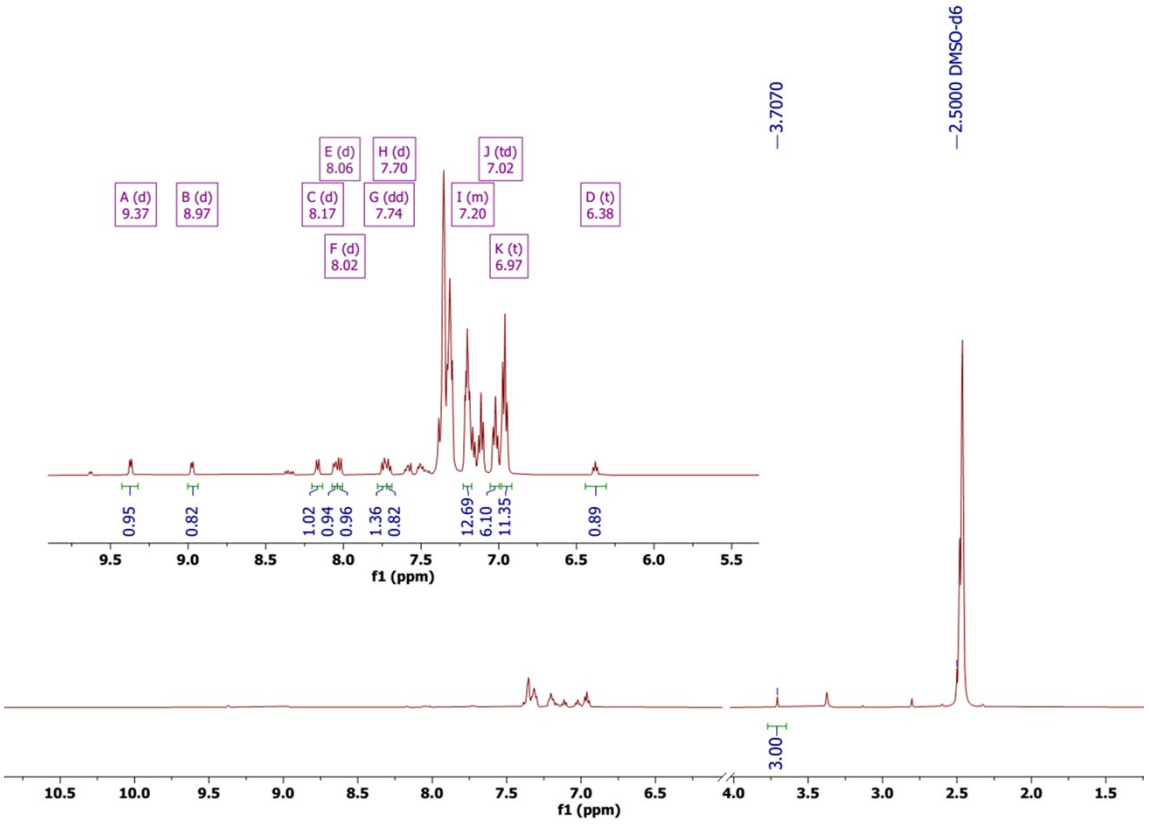

Figure S34. ^{1}H NMR of complex **2c** in DMSO-d_6.

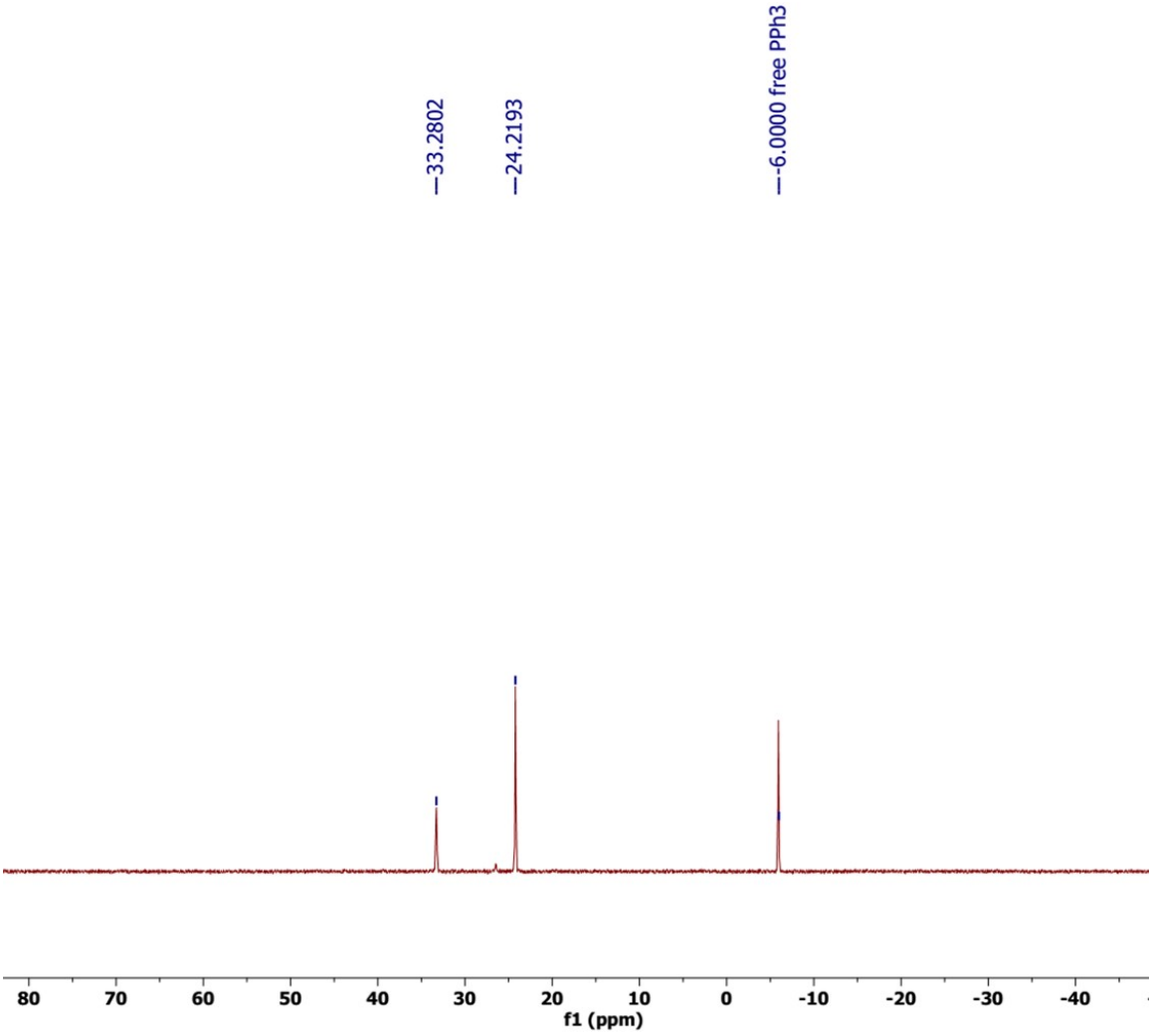

Figure S35. ^{31}P NMR of complex **2c** in DMSO-d_6.

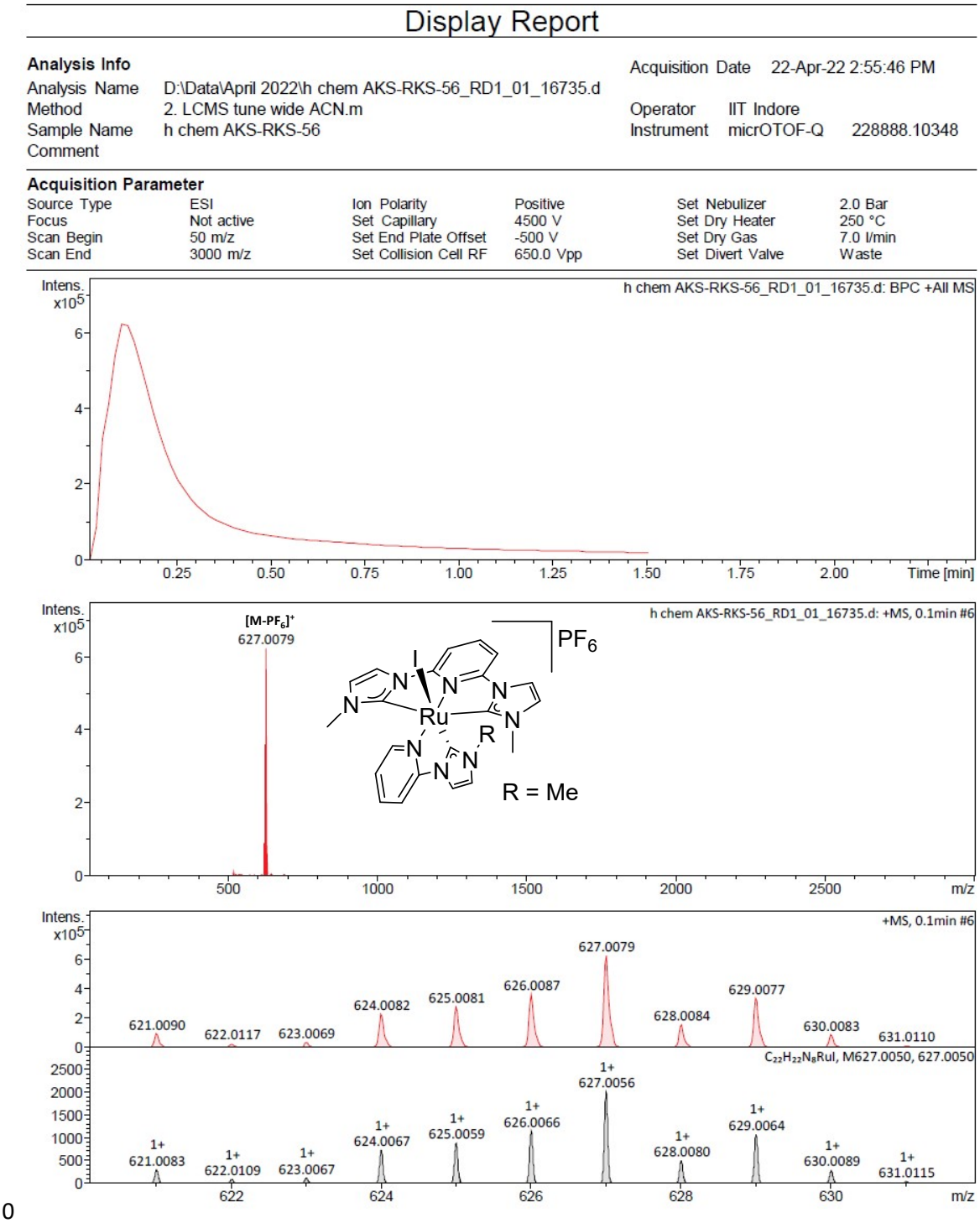

Figure S36. LCMS and HRMS of complex **3a**.

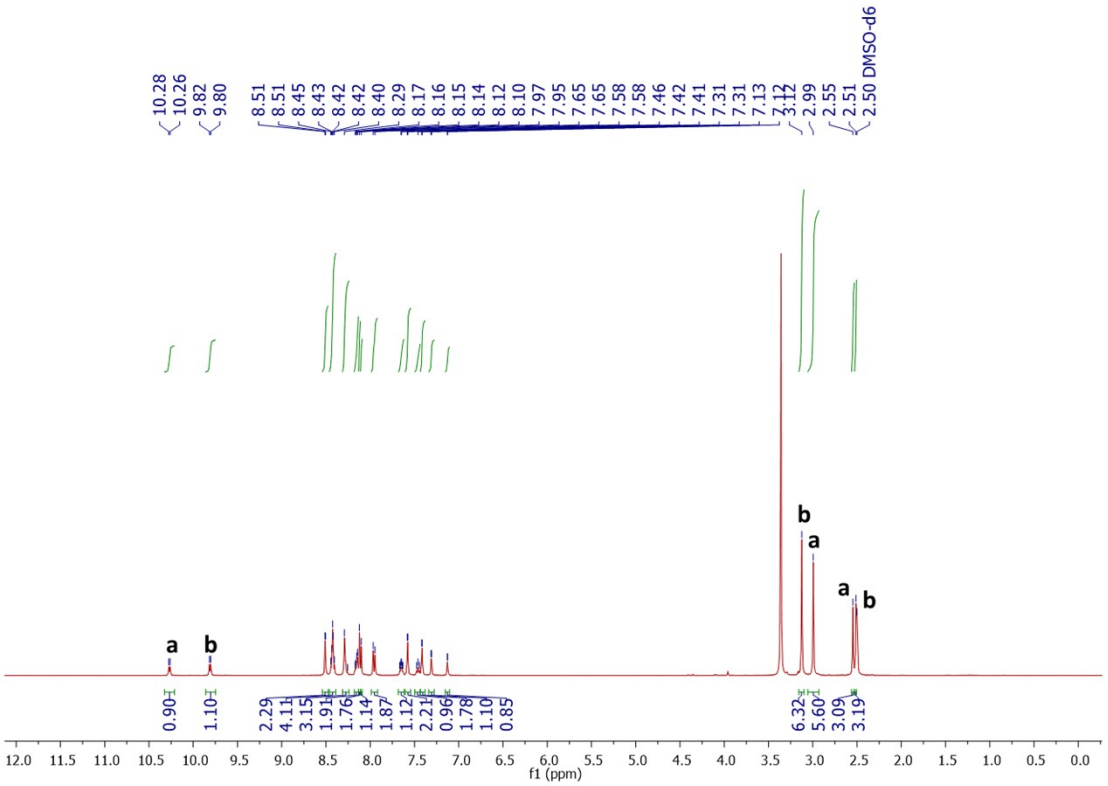

Figure S37. ^{1}H NMR of complex **3a** in DMSO-d_6 showing two distinct species **a** (45%) & **b** (55%) in solution.

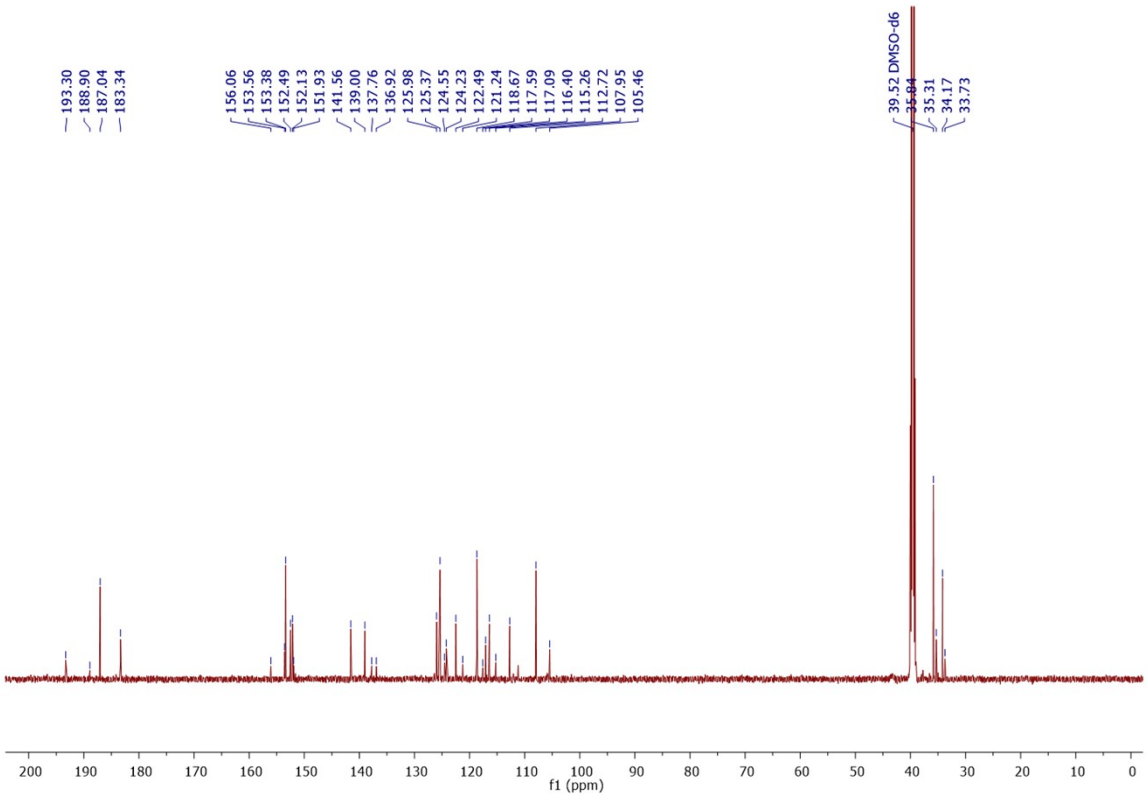

Figure S38. ^{13}C NMR of complex **3a** in DMSO-d_6 showing two distinct species **a** and **b** in solution.

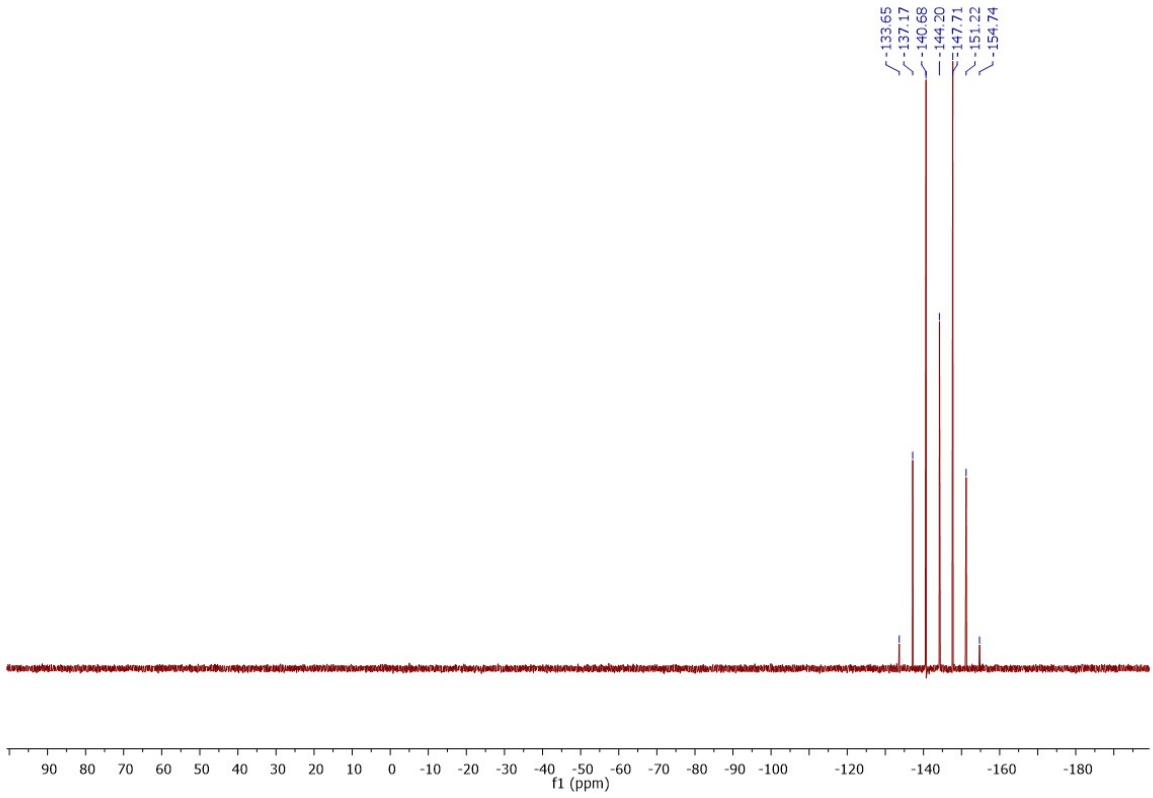

Figure S39. ^{31}P NMR of complex **3a** in DMSO-d_6.

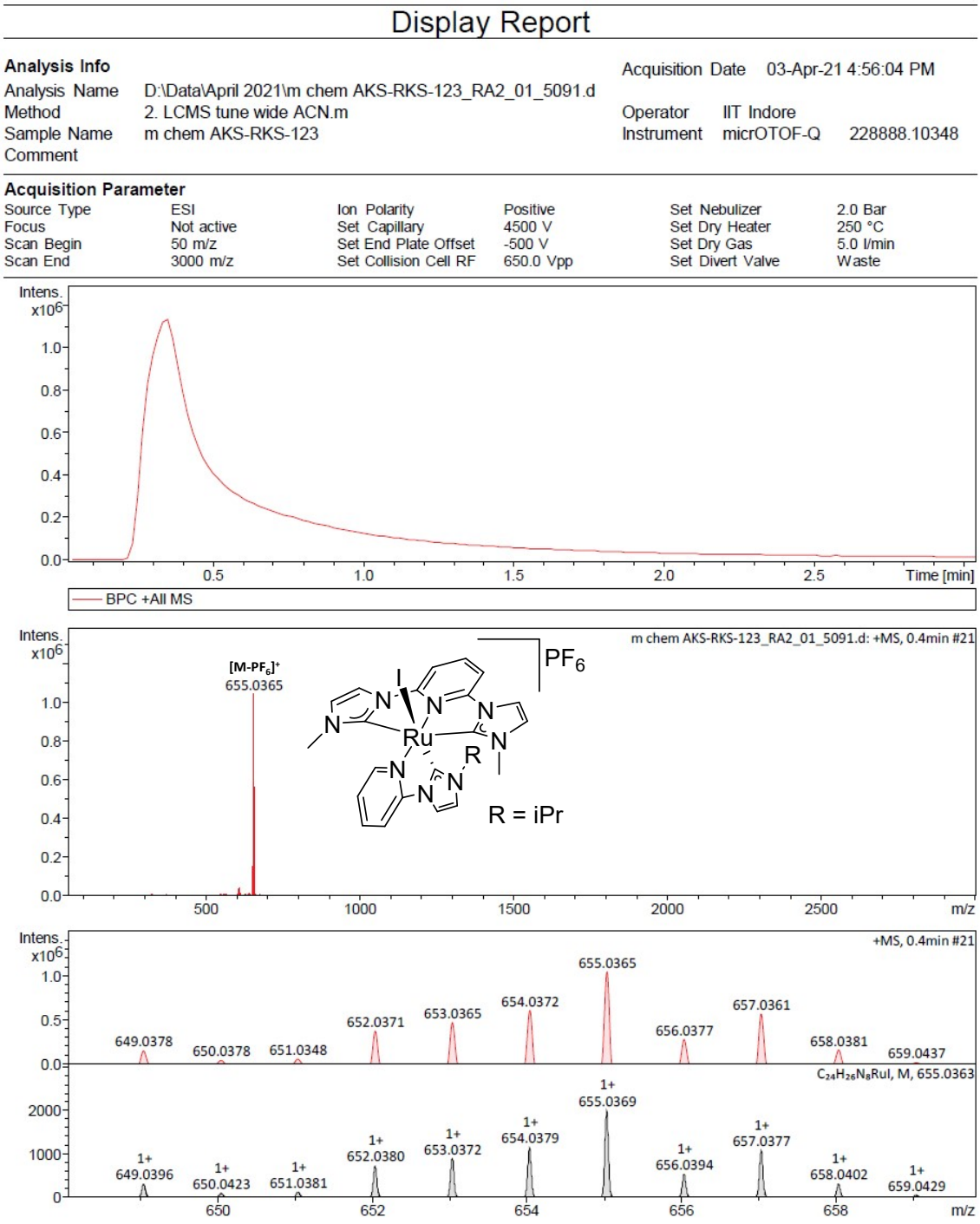

Figure S40. LCMS and HRMS of complex **3b**.

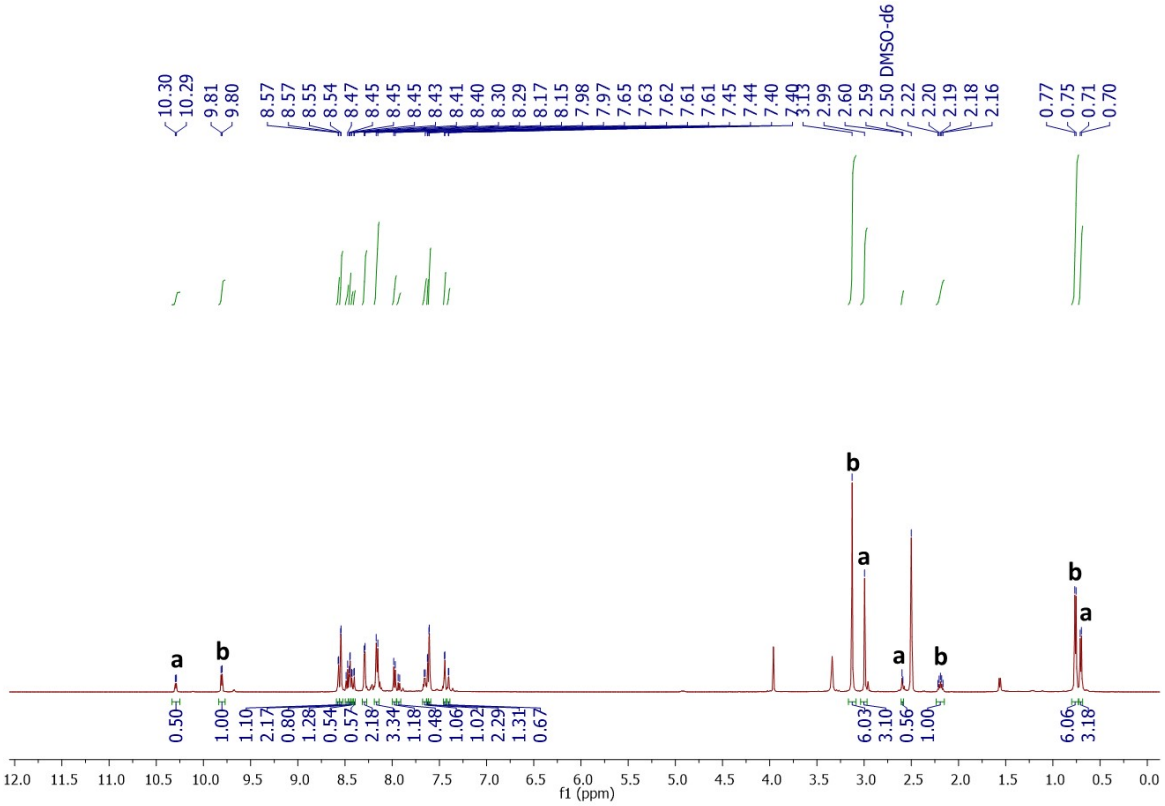

Figure S41. ^{1}H NMR of complex **3b** in DMSO-d_6 showing two distinct species **a** (33%) and **b** (67%) in solution.

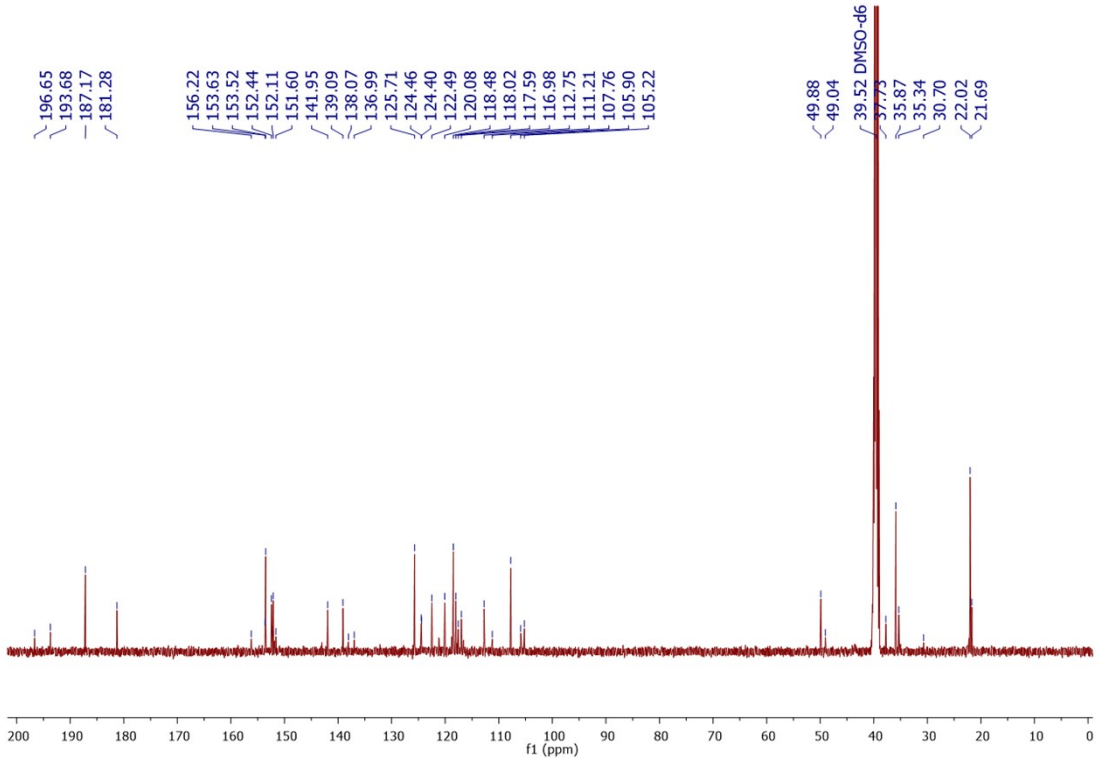

Figure S42. ^{13}C NMR of complex **3b** in DMSO-d_6 showing two distinct species **a** and **b** in solution.

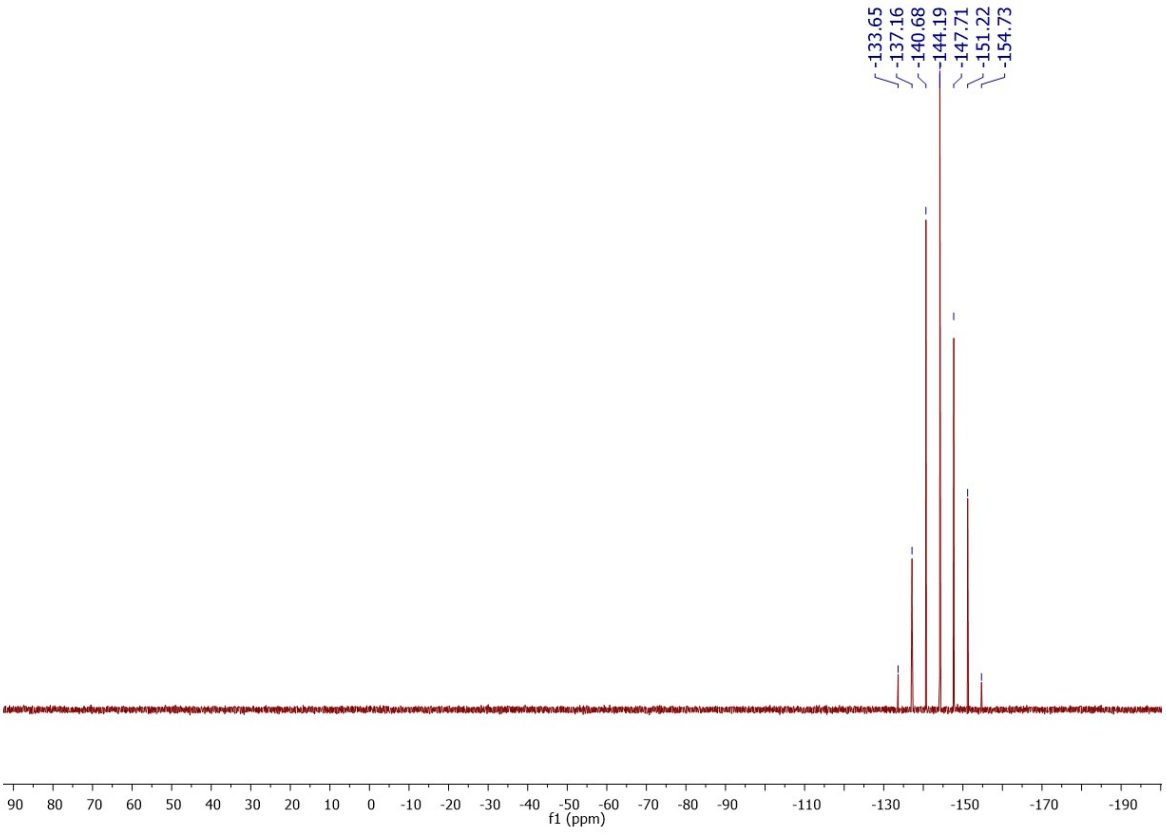

Figure S43. ^{31}P NMR of complex **3b** in DMSO-d_6.

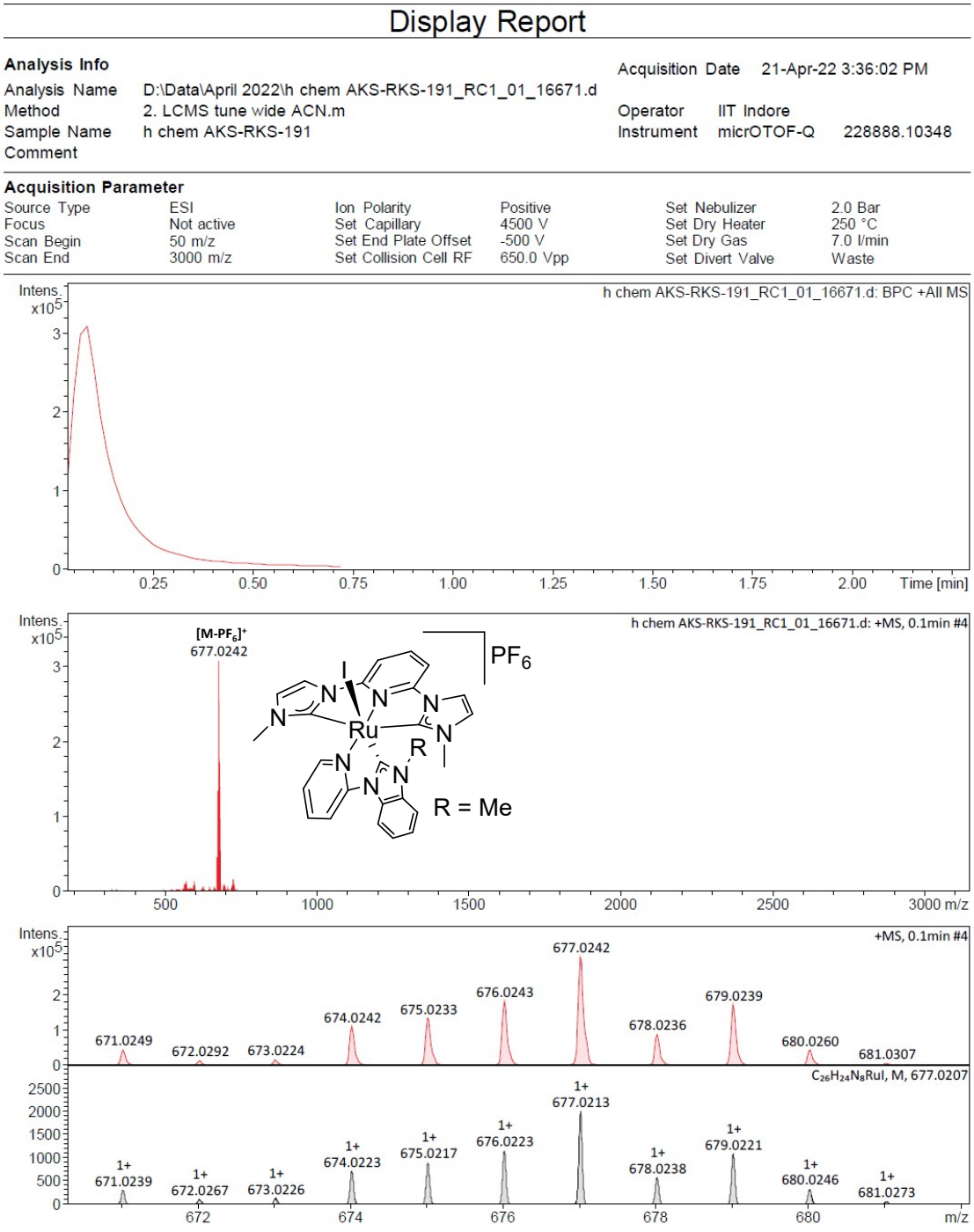

Figure S44. LCMS and HRMS of complex **3c**.

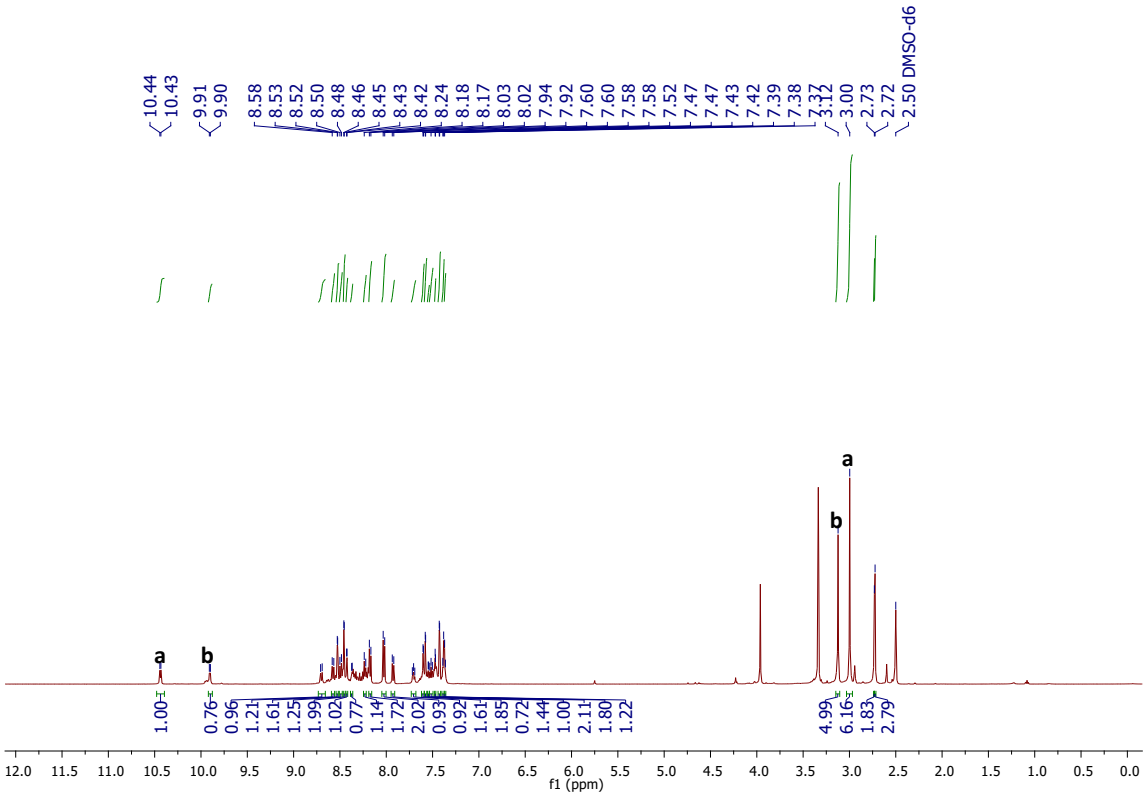

Figure S45. ^{1}H NMR of complex **3c** in DMSO-d_6 showing two distinct species **a** (57%) and **b** (43%) in solution.

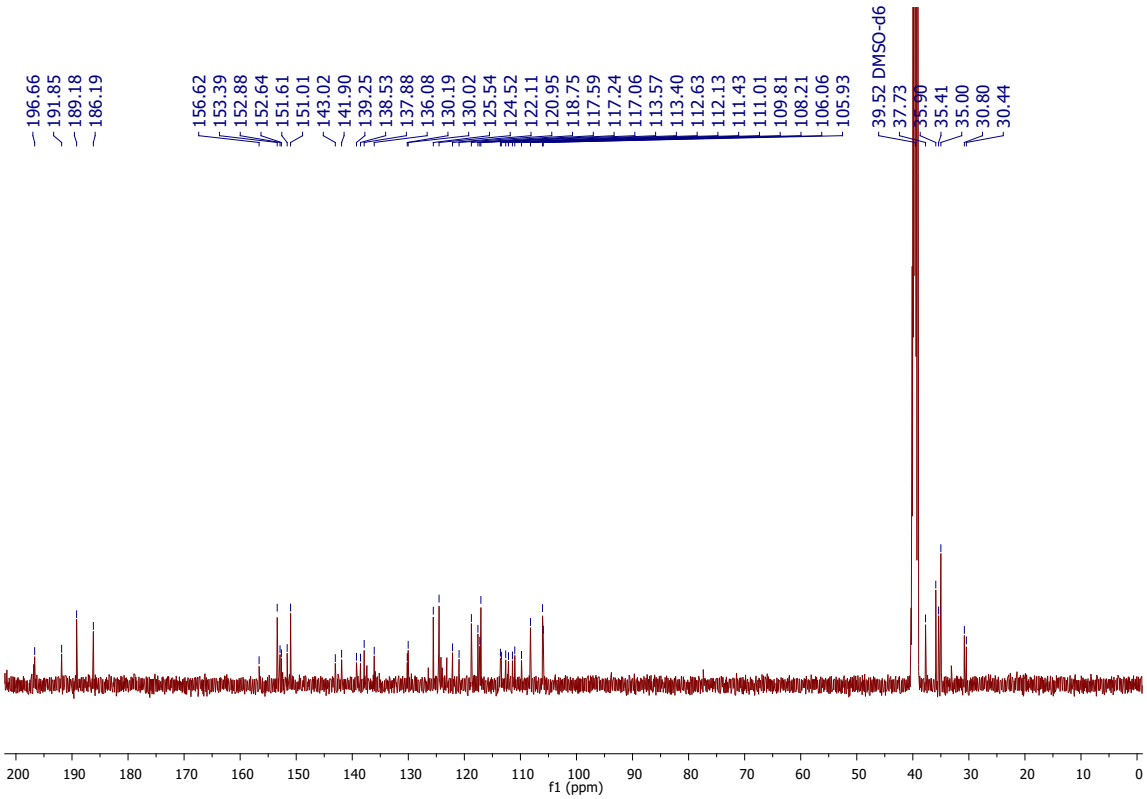

Figure S46. ^{13}C NMR of complex **3c** in DMSO-d_6 showing two distinct species **a** and **b** in solution.

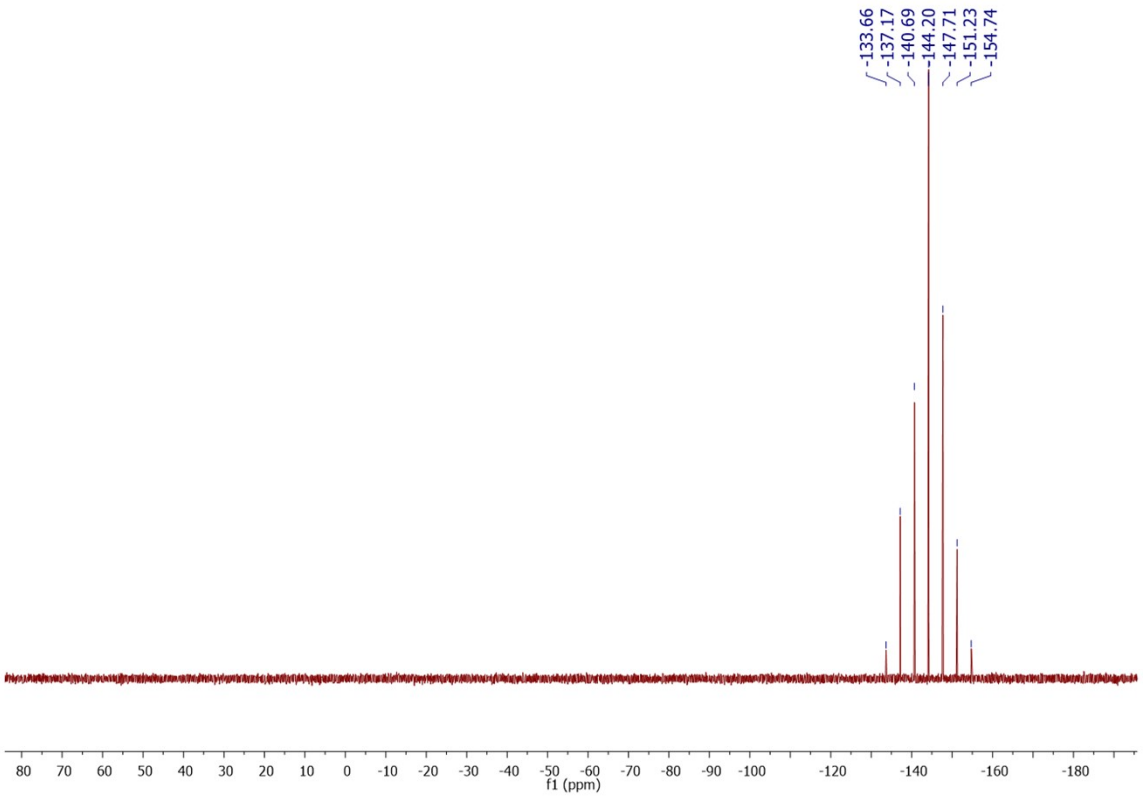

Figure S47. ^{31}P NMR of complex **3c** in DMSO-d_6.

Crystal Structure 3a

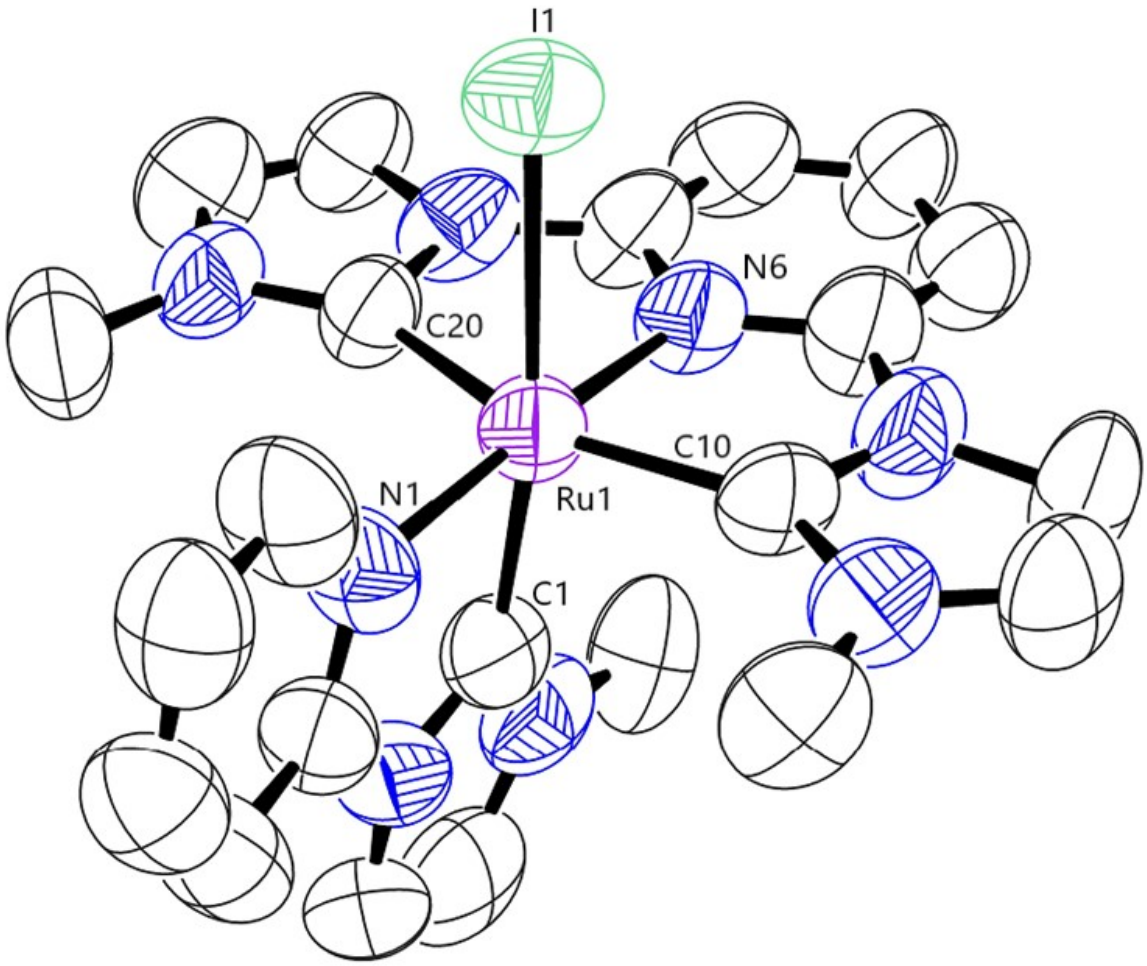

Figure S48. ORTEP diagram for complex **3a** obtained from X-ray diffraction. Hydrogen atoms, and one PF_6^- anion present in the lattice are omitted for clarity. Ellipsoids are shown at the 50% probability level.

Table S1. Crystallographic parameters for complexes **1a**, **1b**, **2c**, and **3a**.

	1a	**1b**	**2c**	**3a**
Empirical formula	$C_{12.50}H_{14.25}Cl_3N_{4.75}Ru$	$C_{13}H_{21}Cl_3N_3O_2Ru$	$C_{55}H_{50}Cl_2N_4P_2Ru$	$C_{22}H_{22}IF_6PN_8Ru$
Fw/g M^{-1}	438.46	458.75	1028.92	771.41
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P12_1/n1$	$P12_1/c1$	$P12_1/c1$	$P12_1/c1$
***a*/Å**	8.1527(5)	10.9711(2)	11.8605(4)	15.0771(5)
***b*/Å**	17.7460(14)	11.9322(2)	23.0124(7)	10.9379(5)
***c*/Å**	12.1658(7)	14.5760(3)	19.4293(6)	16.8084(6)
α/°	90	90	90	90
β/°	104.622(7)	98.992(2)	100.884(4)	104.553(4)
γ/°	90	90	90	90
***V*/ Å^3**	1703.1(2)	1884.68(6)	5207.6(3)	2682.97(19)
Z	4	4	4	4
***T*, K**	293(2)	293(2)	293(2)	293(2)
ρ_{calcd}/Mg m^{-3}	1.710	1.617	1.312	1.910
λ/Å (Mo/Cu-Kα)	0.7107	0.7107	0.7107	1.54184
Data/restr./param.	3327/0/174	3713/0/205	11693/0/543	4767/0/355
***F*(000)**	870	924	2120	1504
GOOF	1.069	1.074	0.990	1.039
R (int)	0.0867	0.0611	0.0858	0.1243
$R(F_o)$,[a] $I > 2\sigma(I)$ [$wR(F_o)$[b]]	0.0555 [0.1346]	0.0309 [0.0835]	0.0625 [0.1532]	0.1166 [0.3174]
***R* (all data) [*wR* (all data)]**	0.0988 [0.1509]	0.0363 [0.0868]	0.1083 [0.1844]	0.1579 [0.3690]

Table S2. Selected bond lengths and angles for the complexes **1a**, **1b**, **2c,** and **3a.**

Coordinates of optimized geometry of cis/trans isomers of 1a w.r.t solvent molecule (H_2O/MeCN)

Complex	Bond lengths (Å)		Bond Angles (°)	
1a	Ru1-C1	2.002(6)	C1 Ru1 N1	78.1(2)
	Ru1-N1	2.043(5)	C1 Ru1 Cl1	90.26(19)
	Ru1-Cl1	2.3433(19)	C1 Ru1 Cl2	88.38(19)
	Ru1-Cl2	2.3234(19)	C1 Ru1 Cl3	172.35(18)
	Ru1-Cl3	2.4372(17)	C1 Ru1 N4	98.1(2)
	Ru1-N4	2.043(6)	N1 Ru1 Cl1	90.24(15)
			N1 Ru1 Cl2	89.30(15)
			N1 Ru1 Cl3	94.39(14)
			Cl1 Ru1 Cl2	178.63(7)
			Cl1 Ru1 Cl3	91.18(6)
			Cl2 Ru1 Cl3	90.15(7)
			N4 Ru1 N1	176.2(2)
			N4 Ru1 Cl1	89.21(16)
			N4 Ru1 Cl2	91.16(16)
			N4 Ru1 Cl3	89.42(15)
1b	Ru1-C1	1.972(2)	C1 Ru1 N1	78.32(9)
	Ru1-Cl1	2.3399(7)	C1 Ru1 Cl1	89.71(8)
	Ru1-Cl2	2.3441(7)	C1 Ru1 Cl2	93.33(8)
	Ru1-Cl3	2.3501(7)	C1 Ru1 Cl3	103.01(7)
	Ru1-O1	2.2259(18)	C1 Ru1 O1	169.35(9)
	Ru1-N1	2.073(2)	N1 Ru1 Cl1	87.99(6)
			N1 Ru1 Cl2	89.05(6)
			N1 Ru1 Cl3	178.66(6)
			Cl1 Ru1 Cl2	175.25(3)
			Cl1 Ru1 Cl3	92.21(3)
			Cl2 Ru1 Cl3	90.66(3)
			O1 Ru1 N1	92.30(8)
			O1 Ru1 Cl1	84.88(5)
			O1 Ru1 Cl2	91.52(5)
			O1 Ru1 Cl3	86.40(5)
2c	Ru1-C1	1.951(4)	C1 Ru1 N1	78.66(16)
	Ru1-N1	2.079(3)	C1 Ru1 P1	90.89(12)
	Ru1-P1	2.3847(11)	C1 Ru1 P2	90.96(12)
	Ru1-P2	2.4159(11)	C1 Ru1 Cl1	170.80(13)
	Ru1-Cl1	2.4853(10)	C1 Ru1 N4	97.25(16)
	Ru1-N4	2.045(4)	N1 Ru1 P1	91.58(9)
			N1 Ru1 P2	89.20(9)
			N1 Ru1 Cl1	92.17(9)
			Cl1 Ru1 P1	90.17(4)
			Cl1 Ru1 P2	88.07(4)
			Cl1 Ru1 N4	92.17(9)
			N4 Ru1 N1	175.61(13)
			N4 Ru1 P1	86.87(11)
			N4 Ru1 P2	92.47(11)
			N4 Ru1 Cl1	91.93(10)
3a	Ru1-C10	2.041(12)	C10 Ru1 N6	76.9(5)
	Ru1-C20	2.053(15)	C10 Ru1 C20	154.7(6)
	Ru1-C1	2.001(13)	C10 Ru1 C1	89.7(6)
	Ru1-N6	2.002(11)	C10 Ru1 N1	104.3(5)
	Ru1-N1	2.111(12)	C10 Ru1 I1	86.8(3)
	Ru1-I1	2.8185(14)	N6 Ru1 C20	77.8(5)
			N6 Ru1 C1	98.6(6)
			N6 Ru1 I1	87.9(3)
			C20 Ru1 C1	94.6(6)
			C20 Ru1 N1	101.0(6)
			C20 Ru1 I1	91.8(4)
			C1 Ru1 N1	77.5(6)
			C1 Ru1 I1	171.8(5)
			N1 Ru1 I1	96.1(4)
			N1 Ru1 N4	175.8(5)

DFT data of **1a-transH_2O**

M06L

GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S
Total enthalpy ... -2063.55822234 Eh
Total entropy correction ... -0.06592410 Eh -41.37 kcal/mol

Final Gibbs free energy ... -2063.62414644 Eh

For completeness - the Gibbs free energy minus the electronic energy
G-E(el) ... 0.15272180 Eh 95.83 kcal/mol

PBE0

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FINAL SINGLE POINT ENERGY -2063.917404824662
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XYZ coordinates

Ru	-0.71837612082331	-0.21459601135461	-0.25882519044137
Cl	-2.54899603233529	-1.83268568088878	-0.52644359964250
Cl	-1.92569642403652	1.57780558042384	-1.31990324829772
Cl	0.86026867236543	-1.87506052439103	0.36733036205501
N	1.80418097989906	1.64475849055771	-0.50609234605528
O	-0.40838030835742	-0.83020221326230	-2.39622431009464
N	-1.12048317880486	0.34958667279730	1.66382472231000
N	0.71375259851873	1.67884313666868	1.36209211111442
C	0.72560874906069	1.10656986720982	0.10764687124256
C	2.45371667576533	2.53674570588745	0.33931716647388
C	1.77405760930203	2.56379823110582	1.51900344132573
C	2.19528642046651	1.30763433632320	-1.86613589856345
C	-2.37881255670430	0.28703821945718	3.70126301626277
C	-2.14776273971349	-0.13505355007181	2.39803955983990
H	-2.77545548072180	-0.87794699415896	1.89037871581428
H	3.34841483723994	3.07874794323081	0.03369682706928
H	1.96111659207695	3.12704467364483	2.43163676831418

H	3.17606082541185	1.75067818209133	-2.08628718984262
H	2.25738630415627	0.21405181698757	-1.97546456873693
H	1.45490685902275	1.69358666528258	-2.58546363641726
C	-1.52961135668848	1.23852575423752	4.27708693093821
C	-0.29804709431495	1.27259419125793	2.22881326503967
C	-0.46863950194050	1.74334667827710	3.52994592271325
H	0.21729195752453	2.48833214156932	3.94514209791645
H	-1.69168448916520	1.58620680351320	5.30301860912568
H	-3.22220389757170	-0.13302173688943	4.25749446279321
H	-1.03004232679567	-0.19726844125817	-2.81157817476229
H	-0.93481757283658	-1.65812993824816	-2.35188268749442

DFT data of **1a-cisH_2O**

M06L

GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy ... -2063.56671223 Eh
Total entropy correction ... -0.06601080 Eh -41.42 kcal/mol

Final Gibbs free energy ... -2063.63272303 Eh

For completeness - the Gibbs free energy minus the electronic energy
G-E(el) ... 0.15256295 Eh 95.73 kcal/mol

PBE0
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FINAL SINGLE POINT ENERGY -2063.923842037005
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XYZ coordinates

Ru	-0.85526421274169	-0.15213323581588	-0.13108387150991
Cl	-0.56991369923285	-0.86696981654868	-2.38170587228694
Cl	-2.47078120834026	1.51602168266777	-0.71897128102432
Cl	0.32510774954272	-2.01021388289319	0.74627146849665

N	1.65056119221117	1.59216397512193	-0.58676066018054
O	-2.75688568495256	-1.54298701223137	-0.32218443875065
N	-1.12893863636932	0.45396168272929	1.88163735794808
N	0.72667067596543	1.67469401951757	1.37863312935986
C	0.60993084214555	1.07771647908703	0.12390319841249
C	2.38706365448391	2.47606835935774	0.19370527881965
C	1.81825719055024	2.53540867045420	1.42610309938531
C	1.95447862796159	1.26558055109475	-1.97296472865654
C	-2.19256209405049	0.46164409598198	4.02175930228146
C	-2.09827582688875	0.02281194988589	2.70612146816696
H	-2.80453277190717	-0.69814790823033	2.27716419450347
H	3.26269167629377	2.99332381980415	-0.19775255594614
H	2.09665747021637	3.10741455982846	2.30934874659193
H	2.84511397392343	1.83031086666787	-2.28236256867110
H	2.14503797377561	0.18733261362705	-2.08348234492063
H	1.10797607646634	1.52682107448542	-2.62602868267773
C	-1.24575215034035	1.37784934978685	4.49636897668267
C	-0.21307188329231	1.33443592084826	2.34169377208065
C	-0.23612012767279	1.82608622629606	3.65031411185551
H	0.51966942436319	2.53871120437699	3.99478515573107
H	-1.29298218170102	1.74181341621115	5.52868021784787
H	-2.99552444932757	0.08844253134462	4.66414743059392
H	-3.30900319747222	-0.90621332693457	-0.81560887794157
H	-2.42479840360994	-2.13990786652099	-1.01855102619150

DFT data of **1a-transMeCN**

M06L

GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy ... -2119.81574733 Eh
Total entropy correction ... -0.07095122 Eh -44.52 kcal/mol

Final Gibbs free energy ... -2119.88669854 Eh

For completeness - the Gibbs free energy minus the electronic energy
G-E(el) ... 0.17139142 Eh 107.55 kcal/mol

PBE0

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FINAL SINGLE POINT ENERGY -2120.181937998441
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XYZ coordinates

Ru	-0.63797233189048	-0.38791521827584	-0.23153380221345
Cl	-2.43637641388630	-2.03141832189905	-0.27473163215507
Cl	-1.93278512200531	1.38908223760102	-1.21091893779213
Cl	1.04678752559797	-1.90180468714474	0.57574746369130
N	1.76476325397342	1.64913084254578	-0.53829407846366
N	-0.24661564967592	-1.04786661456889	-2.10087822688204
N	-1.09621110220906	0.25646901357356	1.71301674167771
C	-0.12510431527409	-2.20288208587972	-4.43025668302539
N	0.66668227321204	1.66897655222433	1.32172521093403
C	0.73335500980847	1.04612190356866	0.09580725009326
C	2.33344057486089	2.62953334106921	0.26722020101613
C	1.64598703304460	2.64742837070957	1.44164333181265
C	2.18858705525773	1.29768275330902	-1.88268711328661
C	-0.17814848724894	-1.55293994239440	-3.14258397196305
C	-2.33506696597461	0.24493522067725	3.76286297656971
C	-2.08768005289930	-0.23737937059642	2.48177818163191
H	-2.67766619039436	-1.04000505605525	2.01921700883664
H	3.17956838456626	3.23294881659422	-0.06066781270917
H	1.77656963000580	3.26520628318943	2.32838929642242
H	3.04955448545224	1.91710582033994	-2.16956015930670
H	2.47982441752645	0.23582968601140	-1.92151854505142
H	1.36668393166051	1.46980111105134	-2.59614542098389
H	-0.59073492301441	-1.57085918023401	-5.20300626194646
H	0.91460056039057	-2.41148036250206	-4.72851759934474

H	-0.67232528359645	-3.15851084462864	-4.39218606069573
C	-1.53583652779710	1.27161582263391	4.27351607678366
C	-0.32457979176440	1.24878364822180	2.21399829262588
C	-0.50813180800347	1.78723994236530	3.48741112138209
H	0.13867244764376	2.59052763140272	3.85383932053450
H	-1.70920383290577	1.67085047965870	5.27895095959171
H	-3.15113778446074	-0.18620779256819	4.35086287221590

DFT data of **1a-cisMeCN**

M06L

GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S
Total enthalpy ... -2119.81736903 Eh
Total entropy correction ... -0.07163203 Eh -44.95 kcal/mol

Final Gibbs free energy ... -2119.88900106 Eh

For completeness - the Gibbs free energy minus the electronic energy
G-E(el) ... 0.17055597 Eh 107.03 kcal/mol

PBE0

FINAL SINGLE POINT ENERGY -2120.181137445548

Ru	-0.81394724398615	-0.29273095830890	-0.09791471724466
Cl	-0.38086604663995	-1.00431085136015	-2.32219363572755
Cl	-2.38071912989713	1.39913513953738	-0.74736194577259
Cl	0.48114193099840	-2.03775942381082	0.90933052186057
N	1.66204348294775	1.53762667785858	-0.59299430108419
N	-2.46454905323057	-1.73961353569940	-0.23944818707897
N	-1.13311514163423	0.40373293541905	1.89567068831722
C	-4.17561385283049	-3.55150436851901	-0.99018526873194
N	0.69578156311697	1.65701119750959	1.34544883071666

C	0.62587617996321	1.00925934037750	0.11272133470740
C	2.35060731324281	2.47610242476626	0.16762746458515
C	1.75409567931876	2.55926531978722	1.38422313913595
C	2.01549652332359	1.18268682774974	-1.96056142385465
C	-3.23332117913622	-2.54503451335384	-0.56029395704991
C	-2.22491083484546	0.51732166298709	4.02211336774817
C	-2.10115462248219	0.00452028963979	2.73596510795247
H	-2.79005283454844	-0.75309950910350	2.34516200565746
H	3.21580824213191	3.00913787228781	-0.22581371078898
H	1.99339309788337	3.17217114383999	2.25122397522345
H	2.89353767395274	1.77213789527573	-2.26115607529139
H	2.24524546883035	0.10941365607960	-2.03408824059516
H	1.17788206332196	1.39134620540713	-2.64268621467911
H	-3.79940317764162	-4.55807765632397	-0.74885504814339
H	-5.15219133194009	-3.41387314481569	-0.50016479079075
H	-4.32139546362574	-3.48791417635776	-2.08030006194072
C	-1.30633268370115	1.48255845194556	4.45147656365048
C	-0.24840580258687	1.33559465583196	2.31117125628534
C	-0.29989308237944	1.90356311034866	3.58863352997499
H	0.43174469878897	2.65665234063050	3.89691365606049
H	-1.37462809187321	1.90738938760440	5.45909874560716
H	-3.02841434484182	0.16486160276949	4.67559739129096