Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Supporting Materials

# Amberlite IR-120(H) mediated "On water" synthesis of novel anticancer Ruthenium (II)-p-cymene 2-pyridinylbenzothiazole (BTZ), 2-pyridinylbenzoxazole (BOZ) & 2-pyridinylbenzimidazole (BIZ) scaffolds

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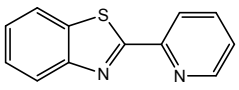


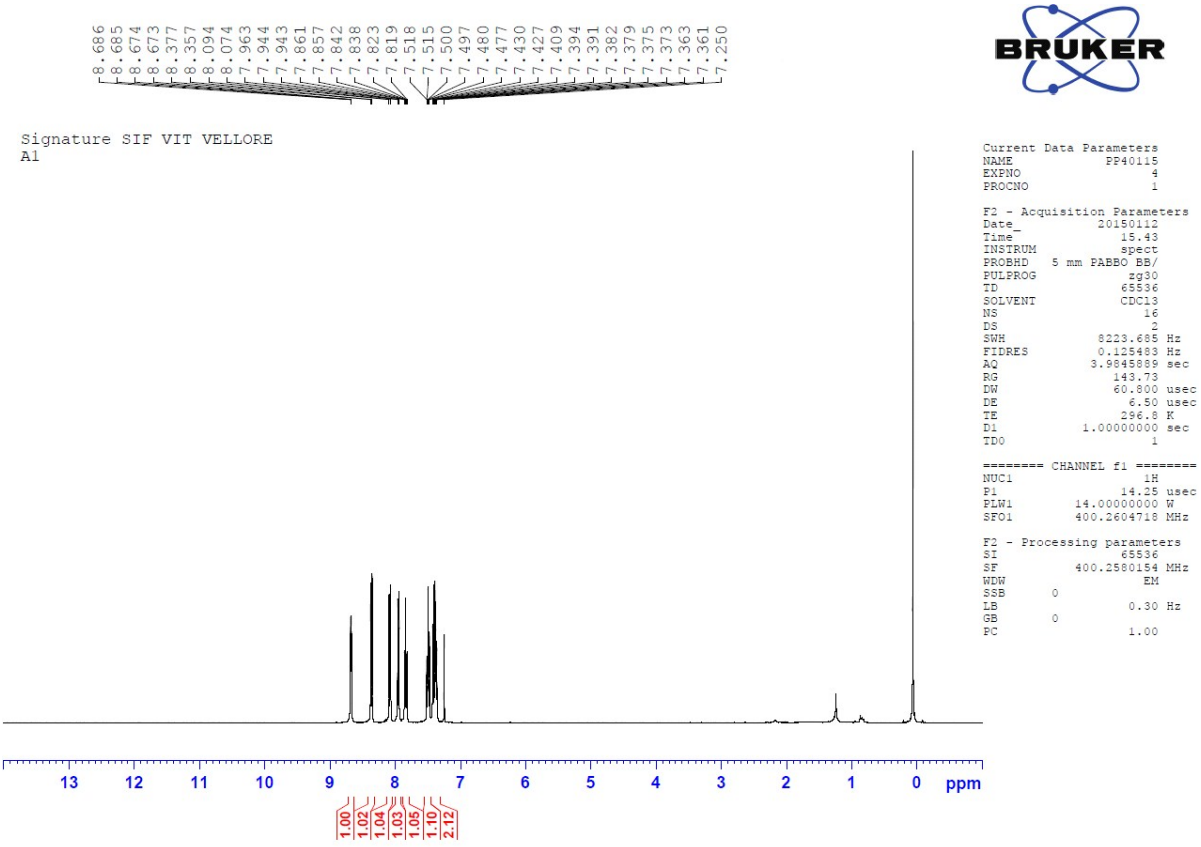




**Figure S1-**$^{1}$H NMR of ligand **3a**

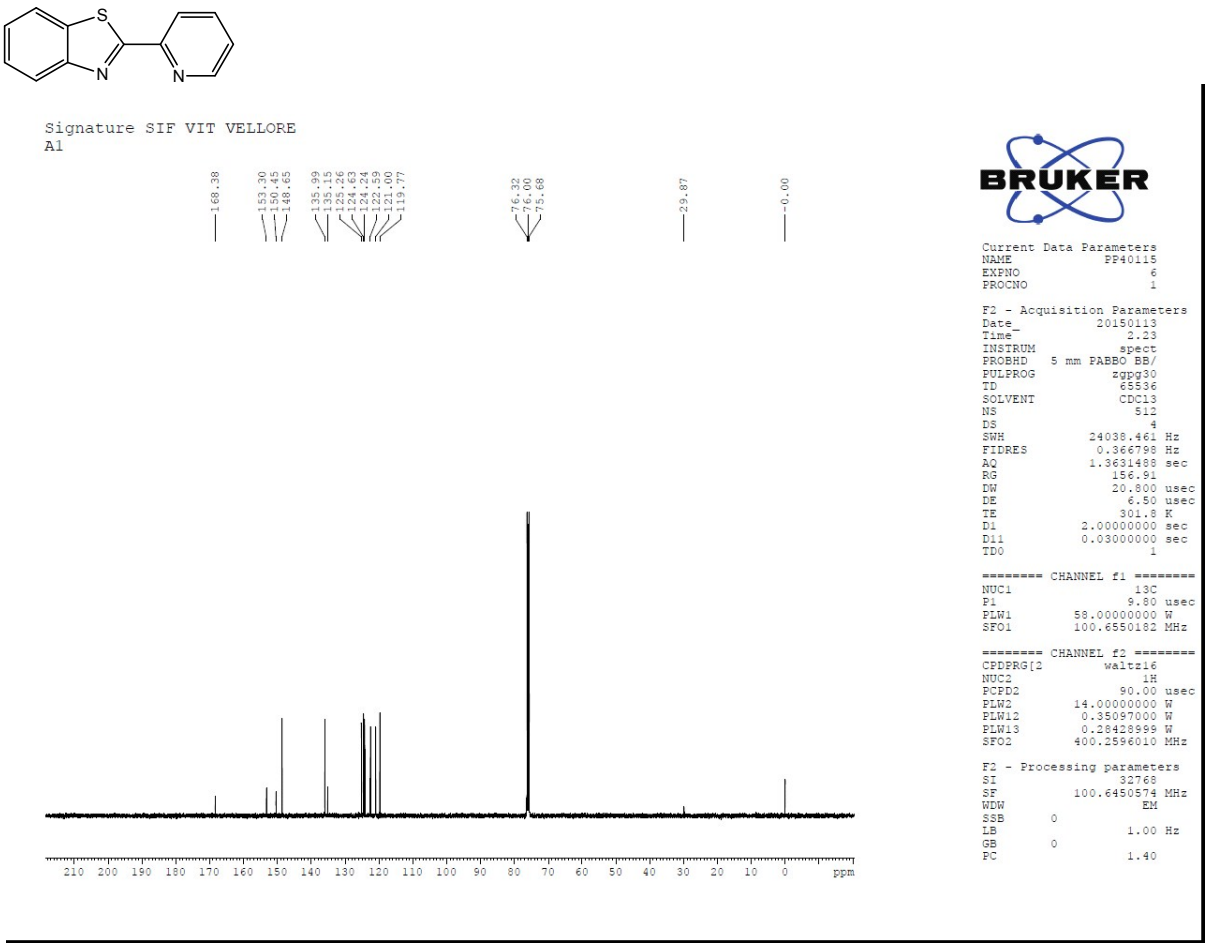
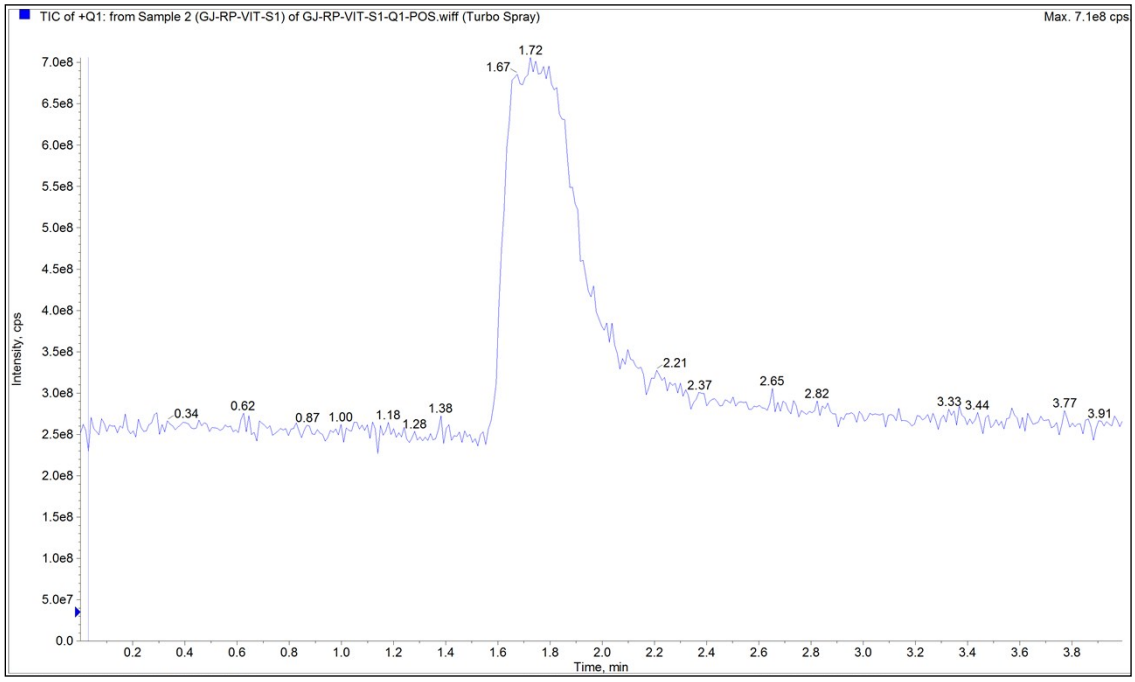



**Figure S2-** $^{13}$C NMR of ligand **3a**

1) TOTAL ION CHROMATOGRAMS (TIC) of ligand **3a**

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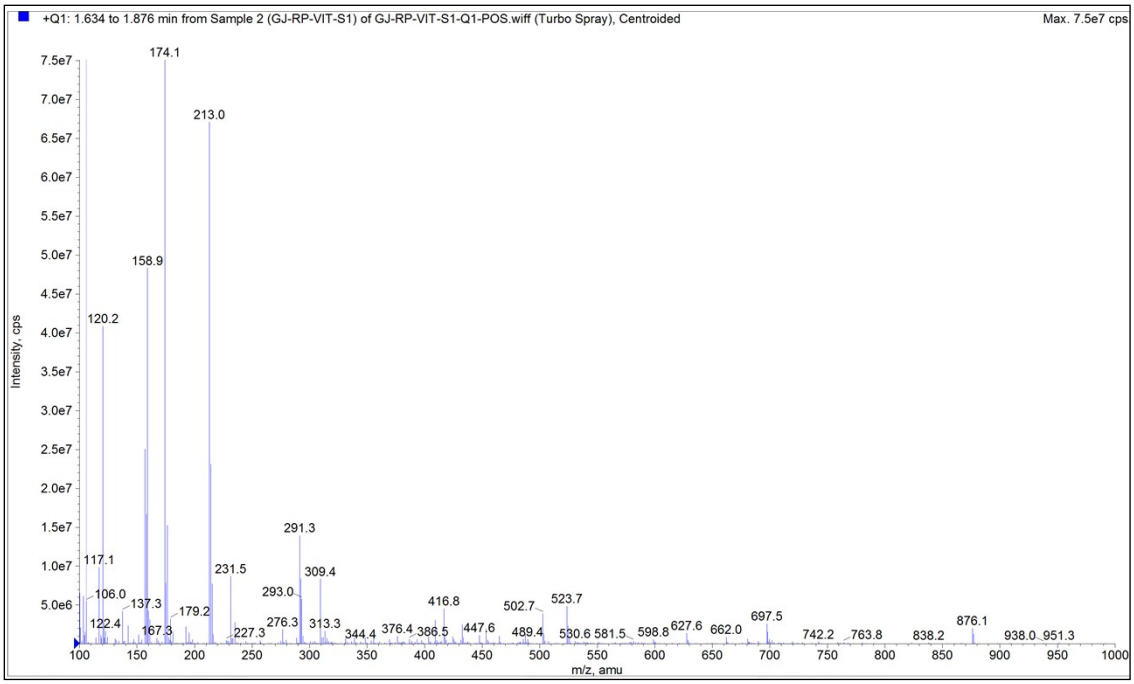



**Figure S3-** MS data for compound **3a**

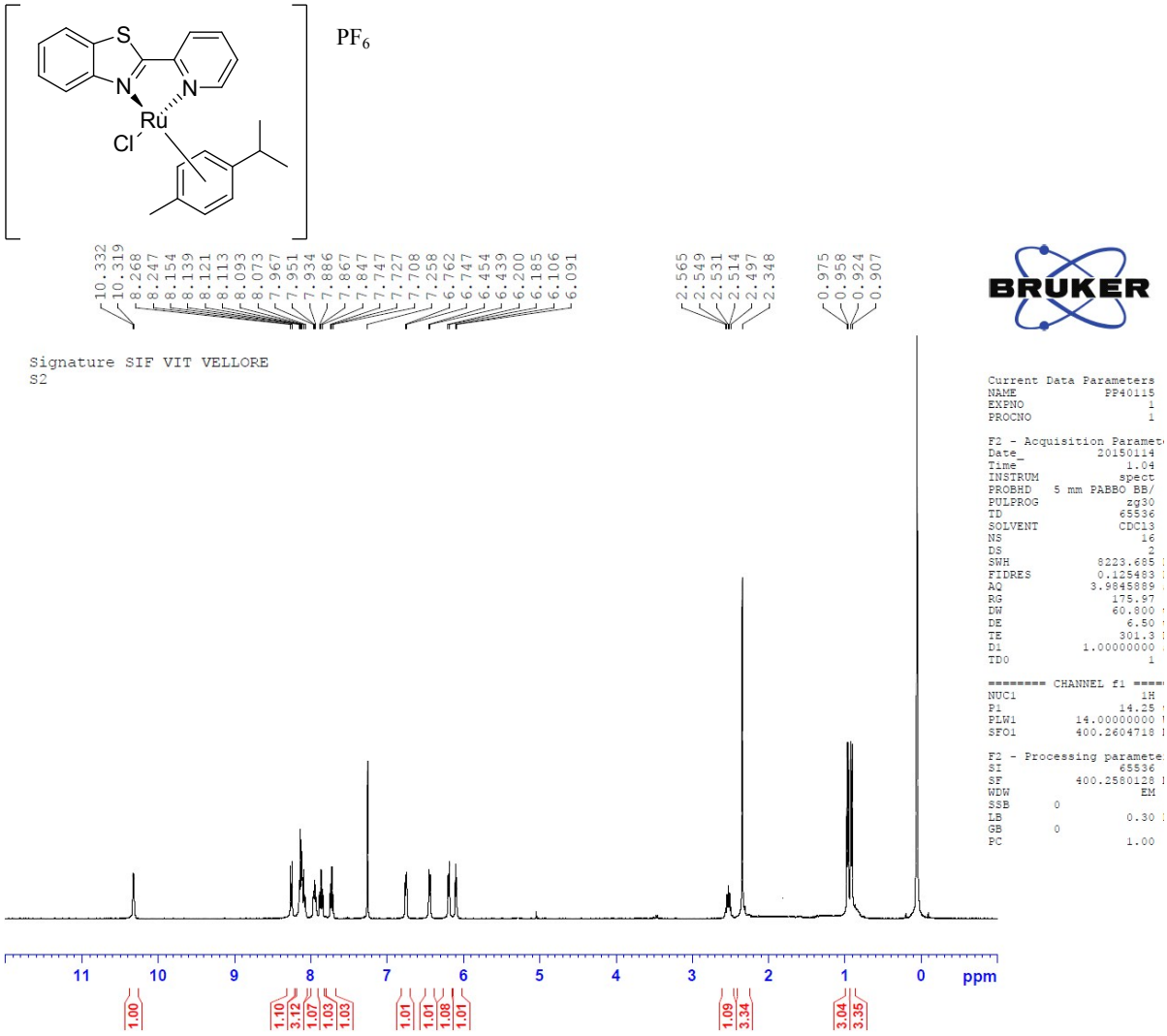



**Figure S4-** $^{1}$H NMR of complex **4a**

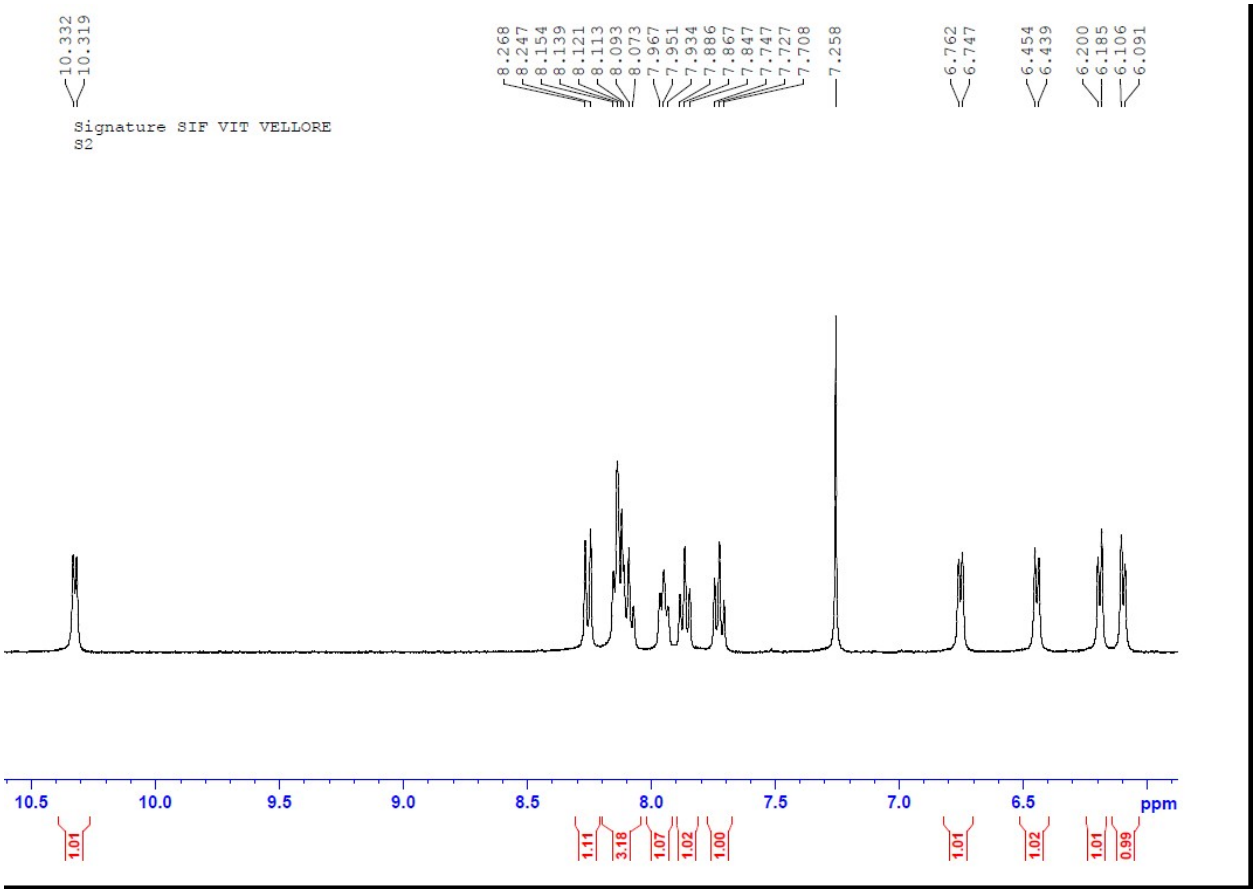
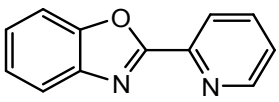



**Figure S5-** $^{1}$H NMR of complex **4a** (Expansion)



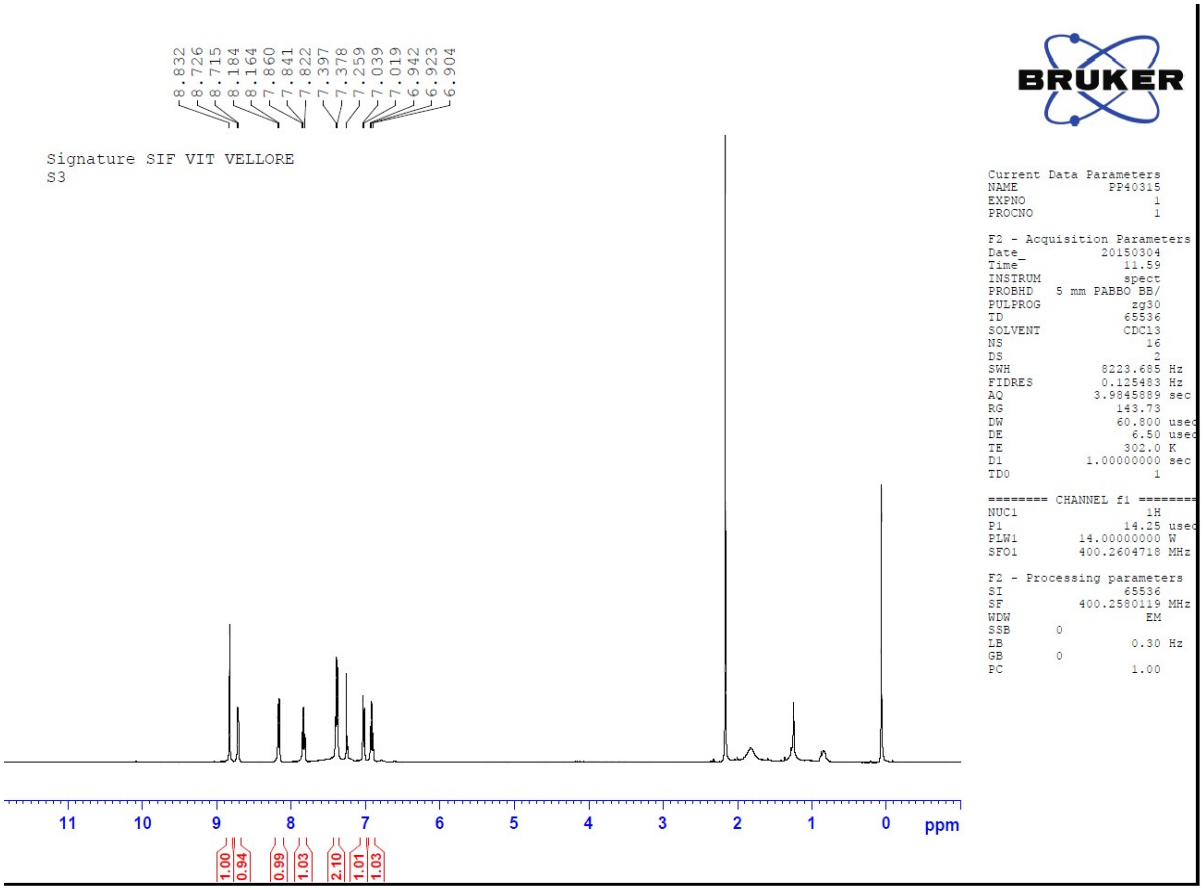



**Figure S6-** $^{1}$H NMR of ligand **3b**

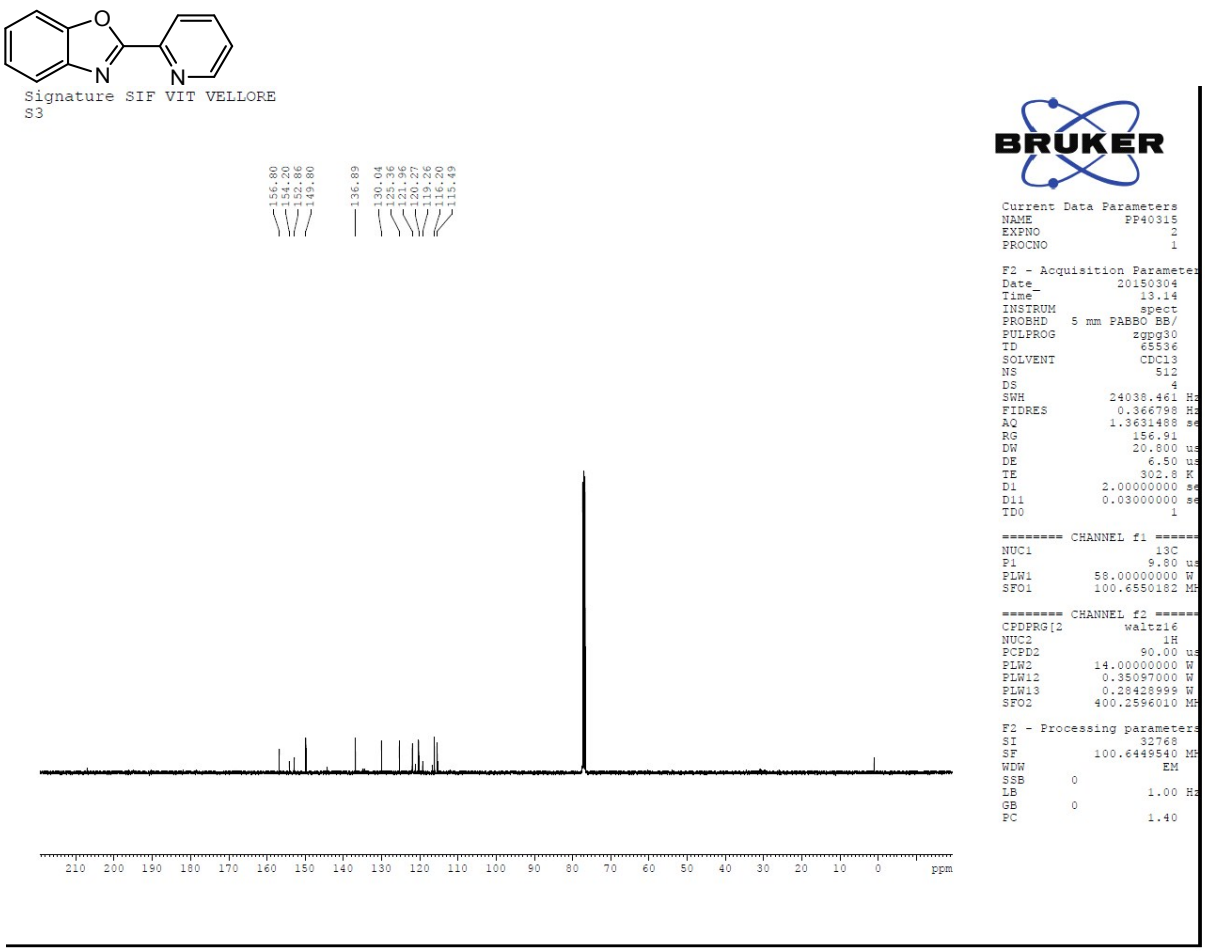



**Figure S7-** $^{13}$C NMR of ligand **3b**

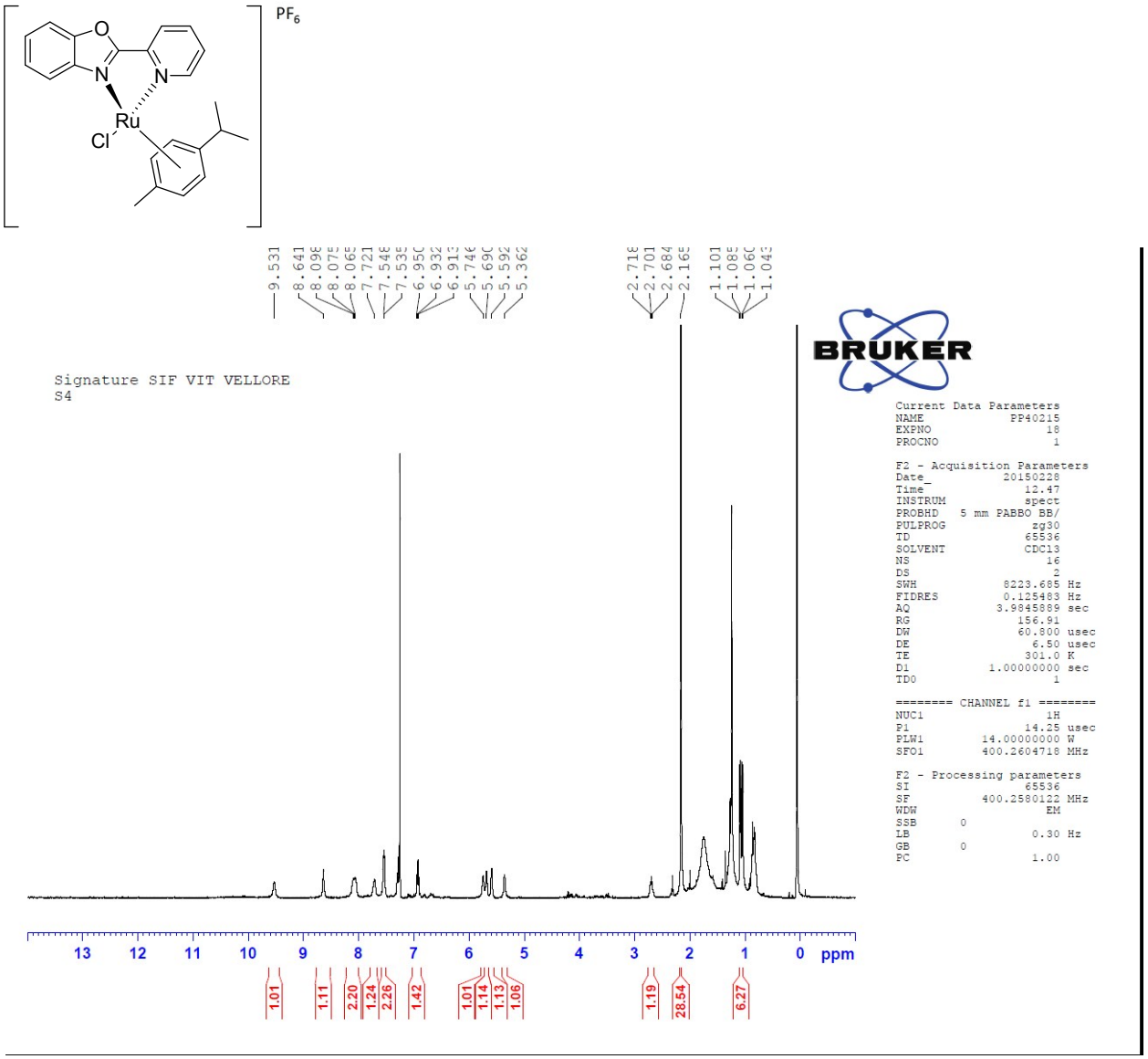



**Figure S8-** $^{1}$H NMR of complex **4b**

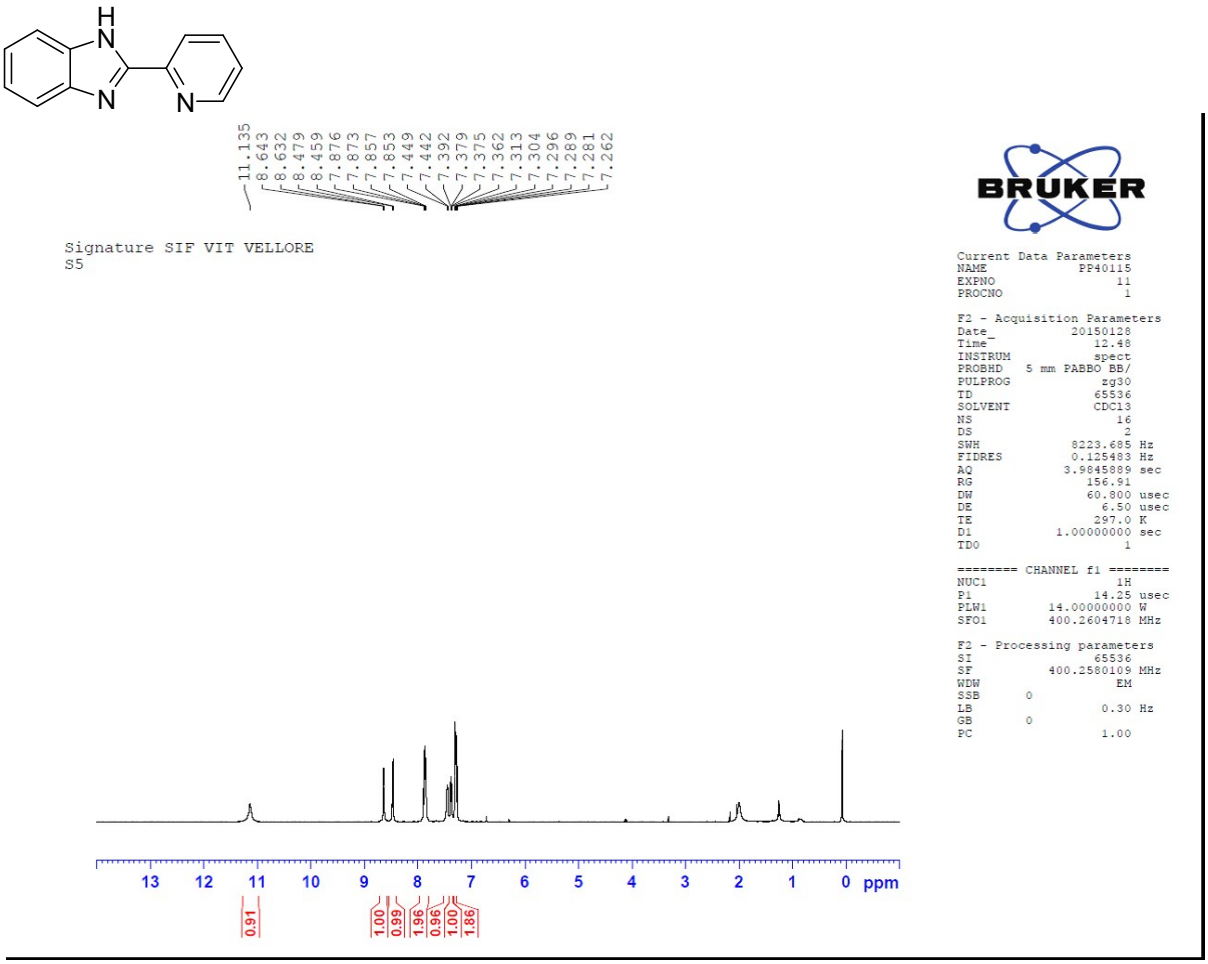



**Figure S9-** $^{1}$H NMR of ligand **3c**

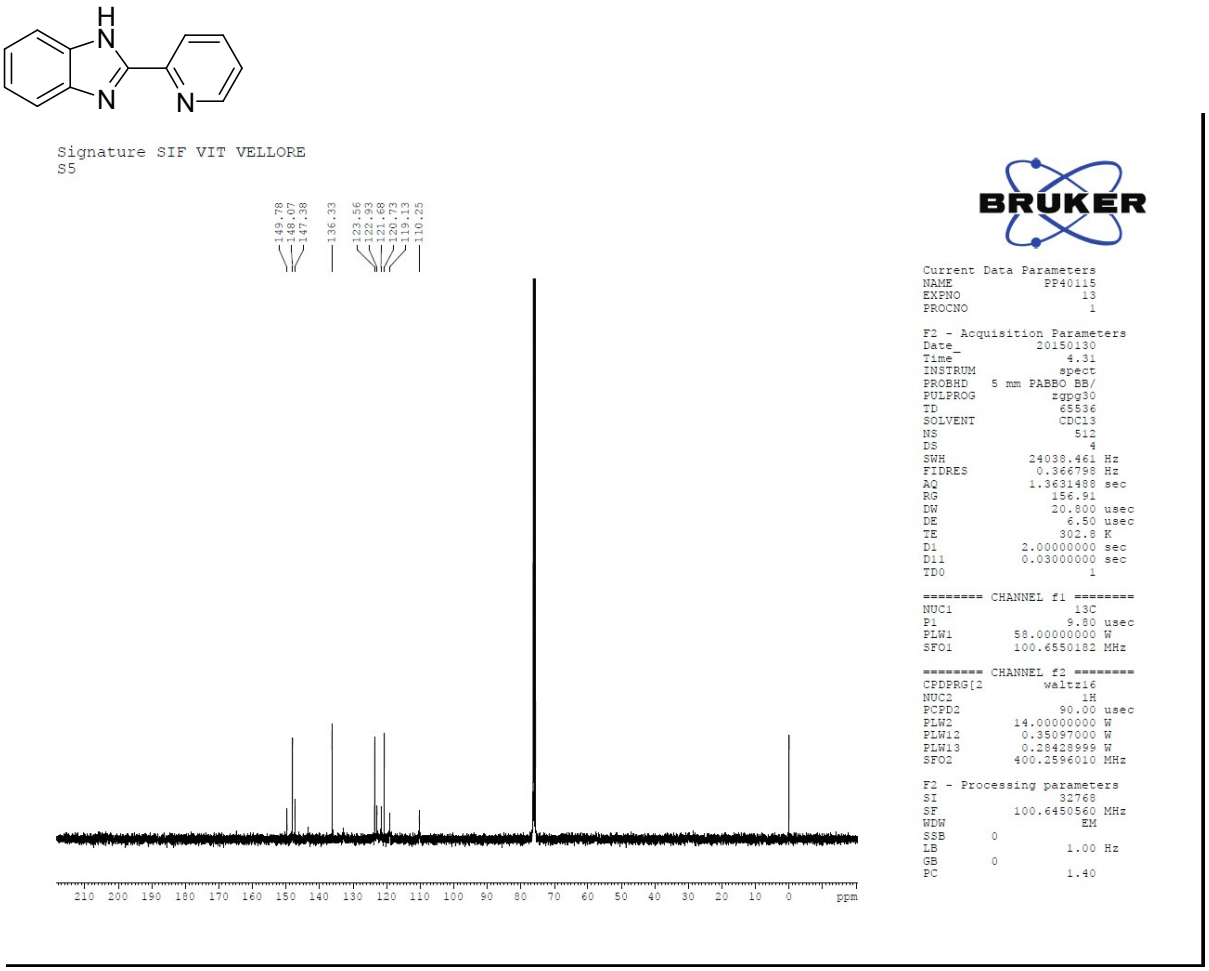



**Figure S10-** $^{13}$C NMR of ligand **3c**

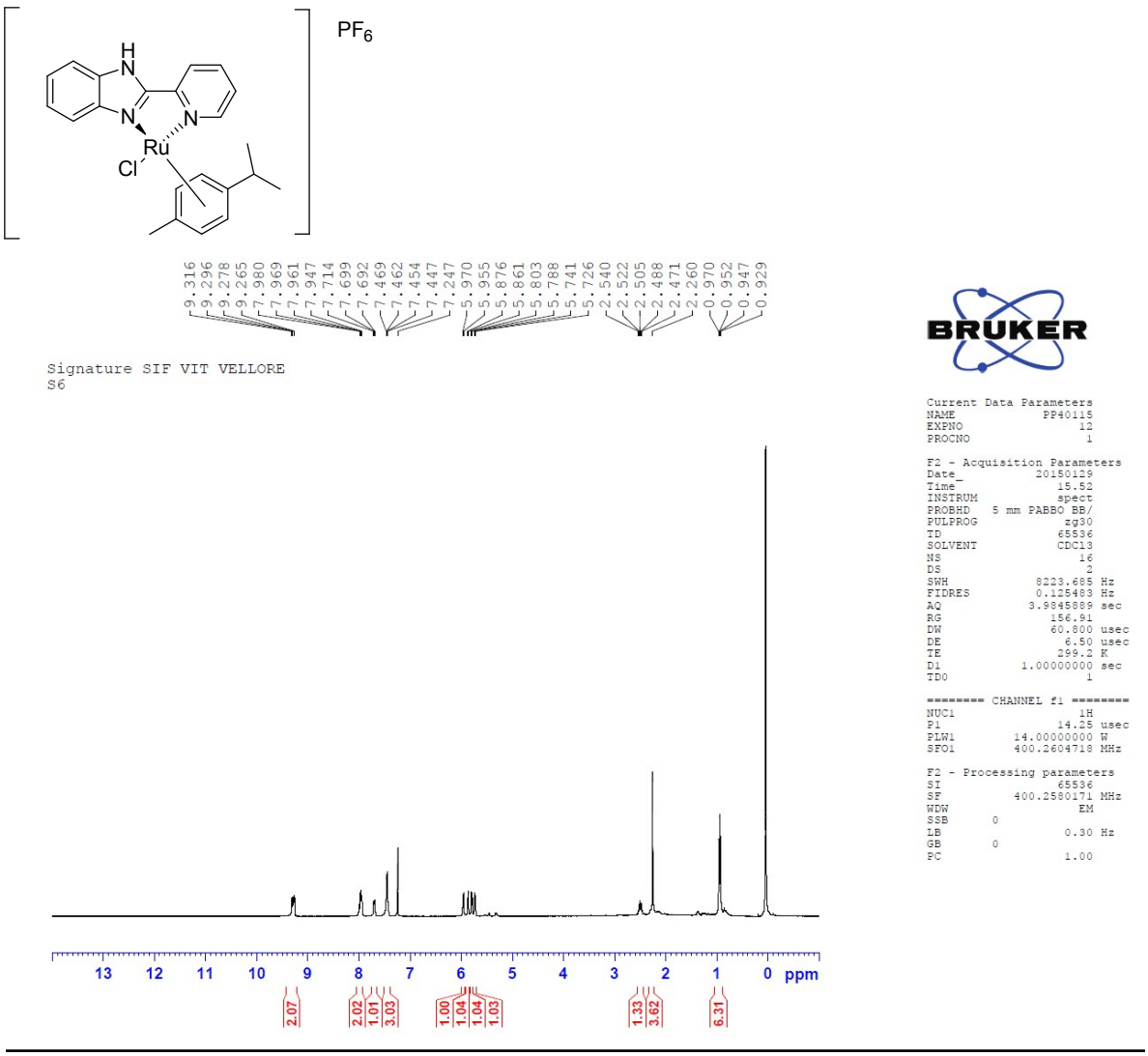



**Figure S11-** $^{1}$H NMR of complex **4c**

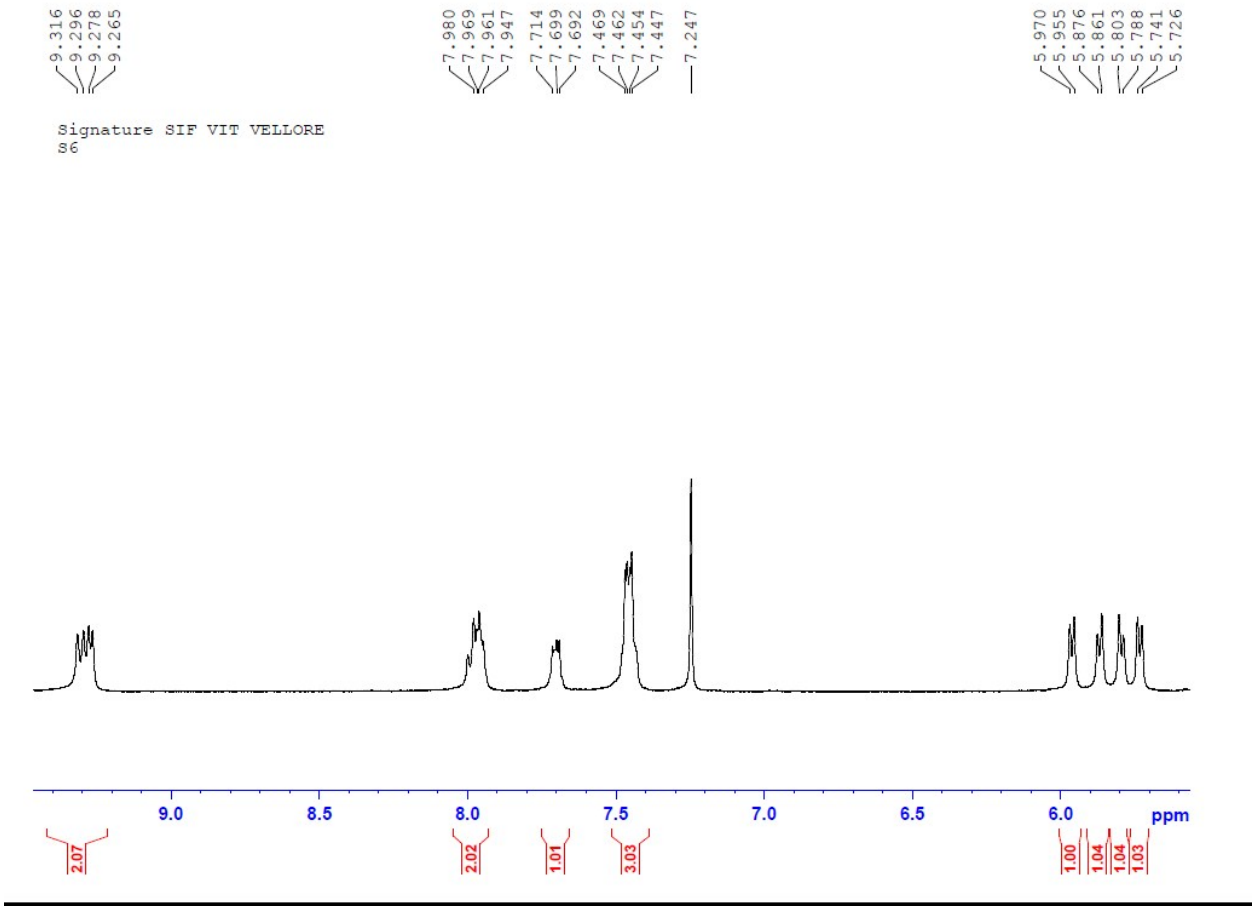



**Figure S12-** $^{1}$H NMR of complex **4c** (Expansion)

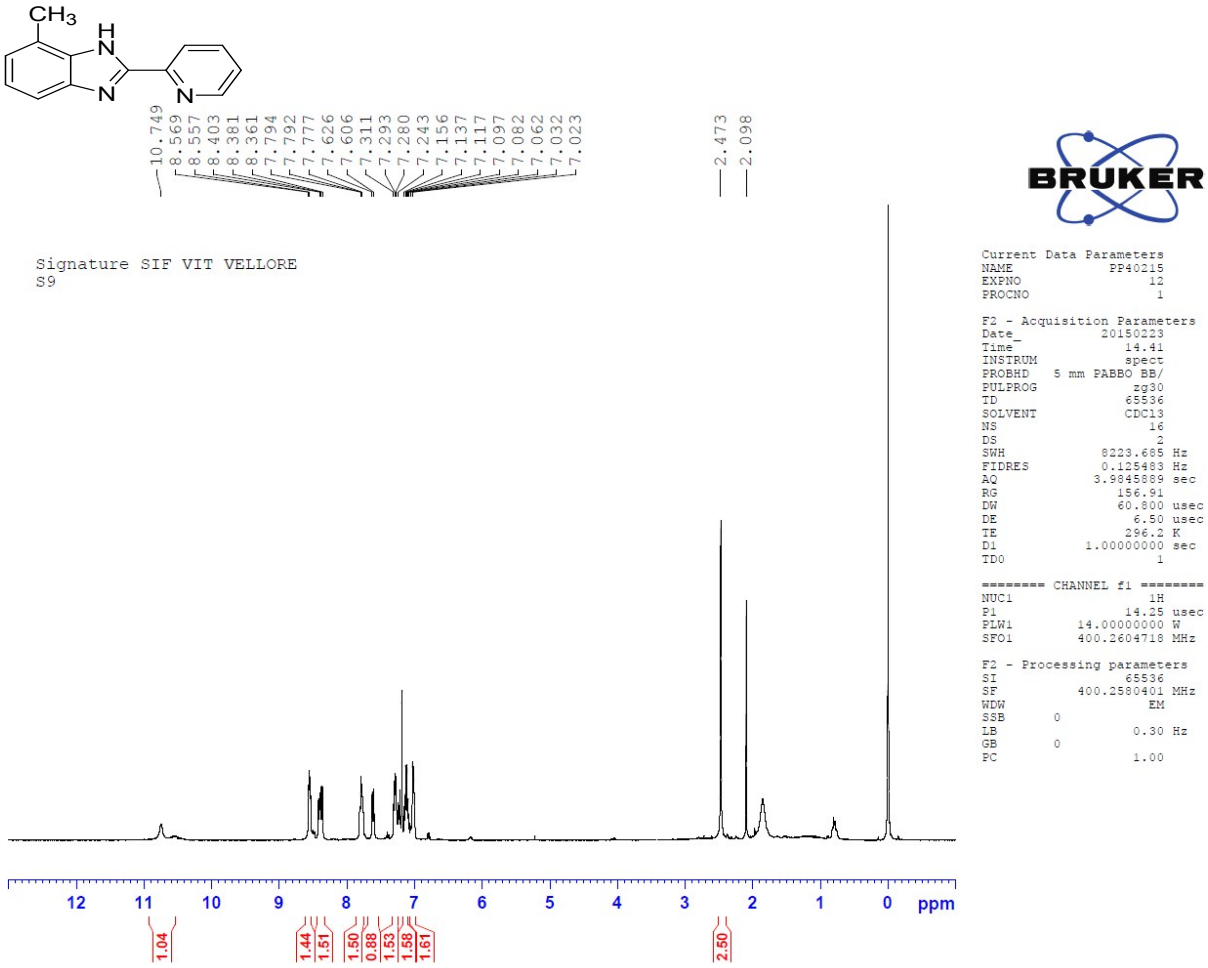



**Figure S13-** $^{1}$H NMR of ligand **3d**

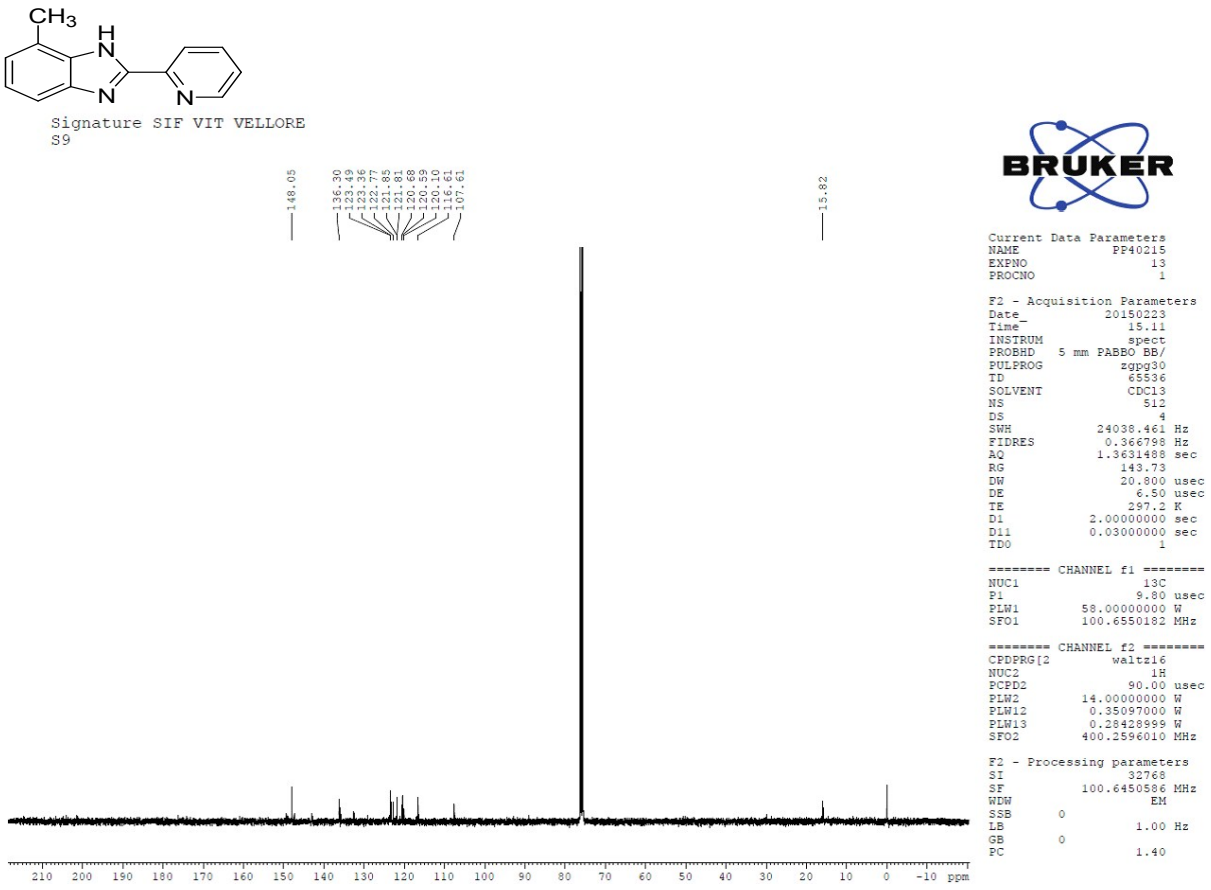



**Figure S14-** $^{13}$C NMR of ligand **3d**

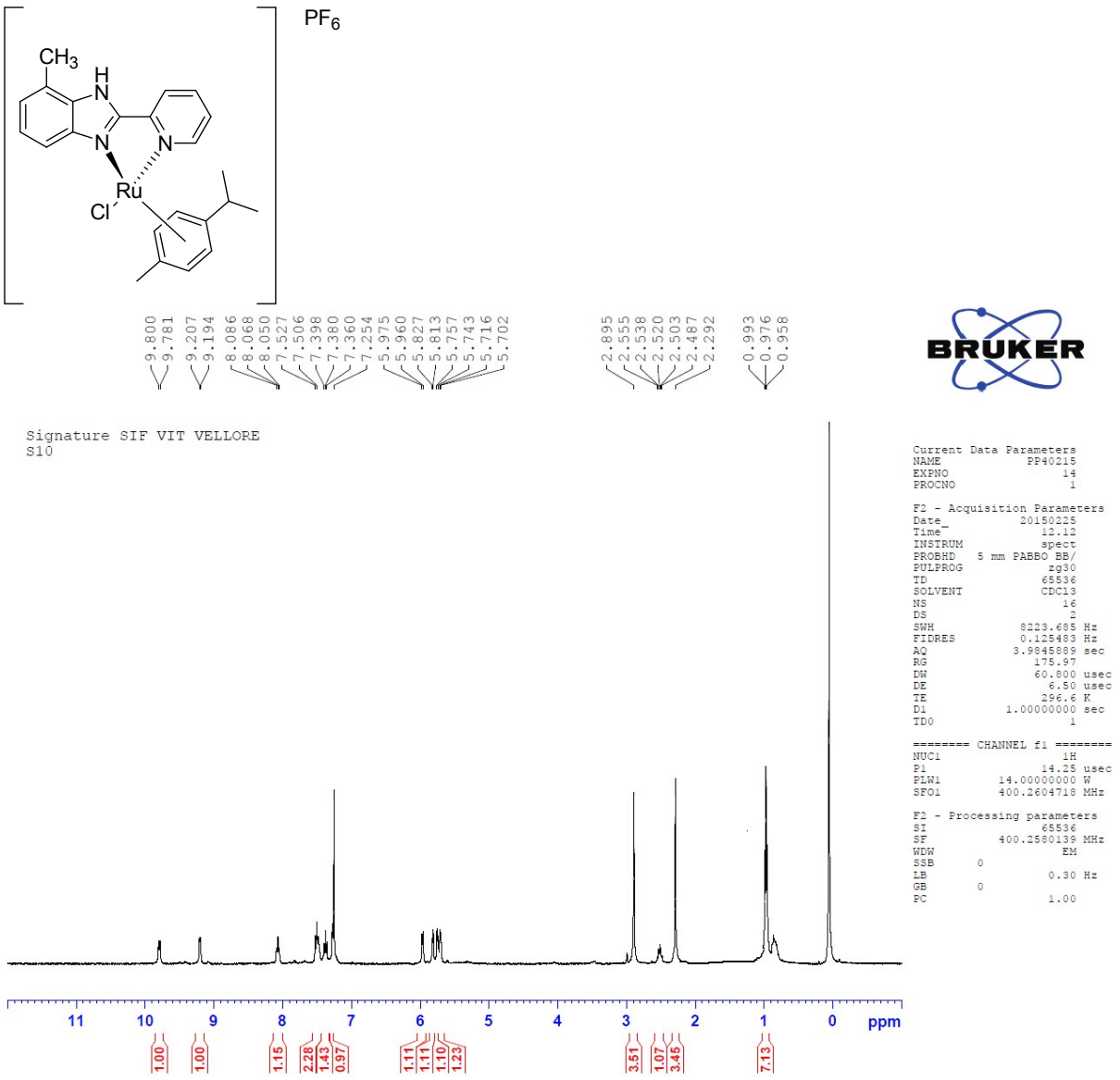



**Figure S15-** $^{1}$H NMR of complex **4d**

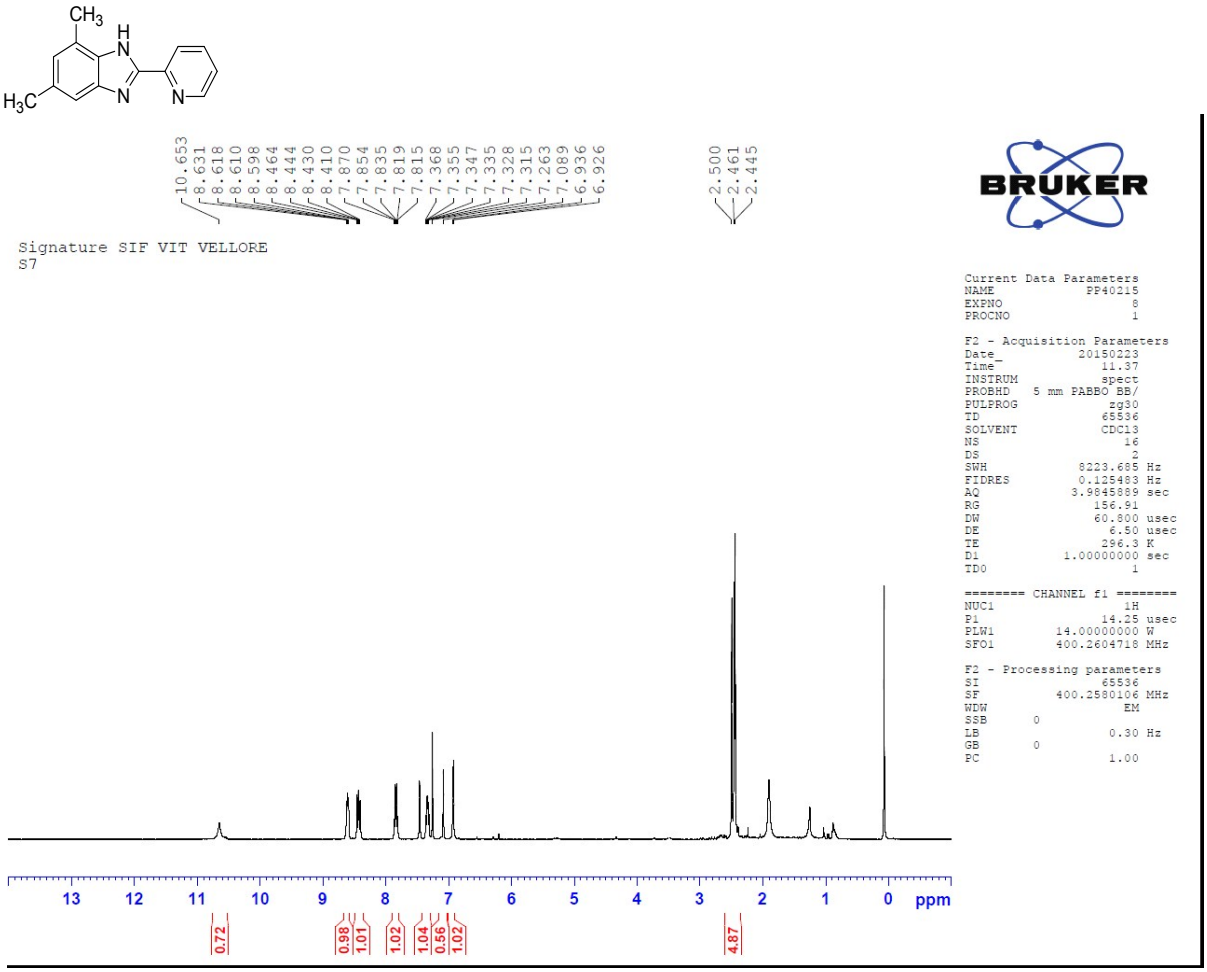



**Figure S16-** $^{1}$H NMR of ligand **3e**

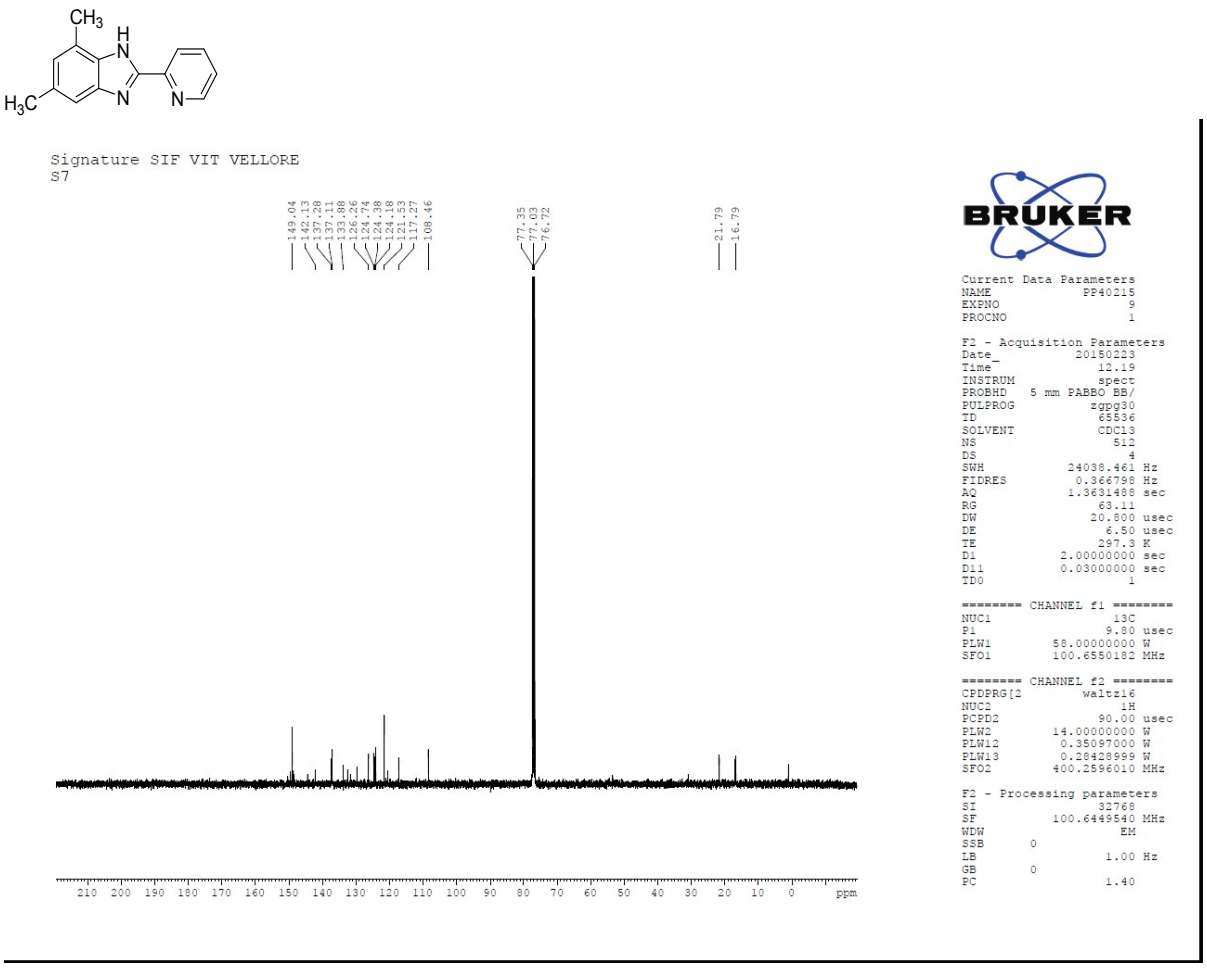
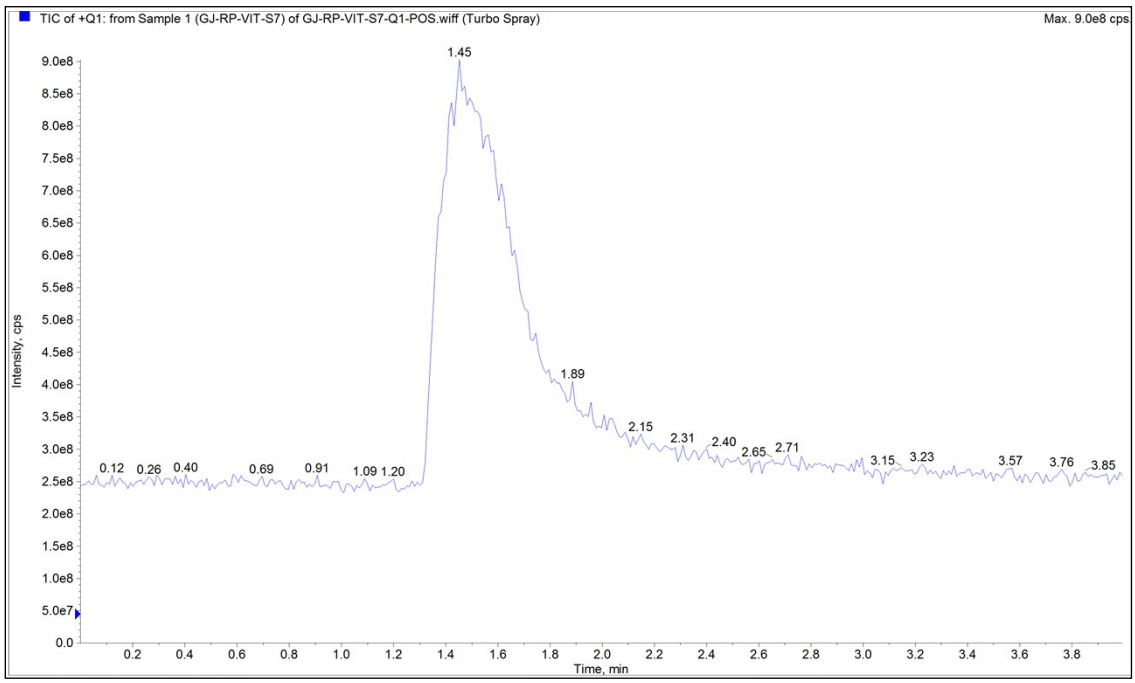



**Figure S17-** $^{13}$C NMR of ligand **3e**

TOTAL ION CHROMATOGRAMS (TIC)




1) MOLECULAR ION (Q1) FOR 224

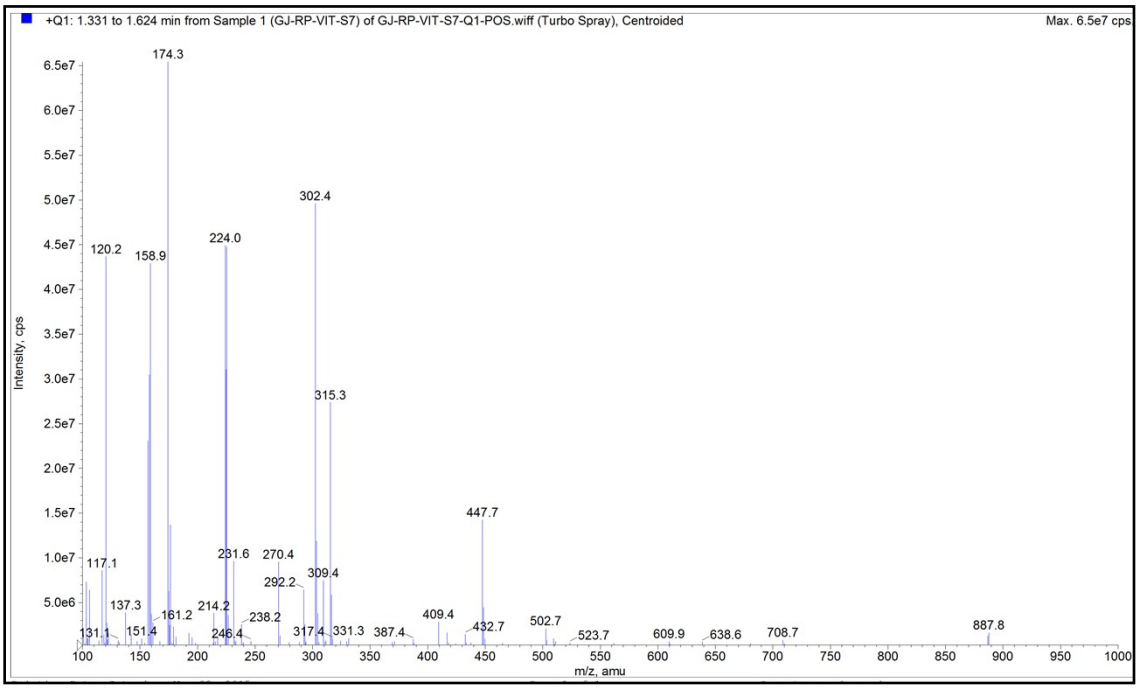



**Figure S18-** MS data for compound **3e**

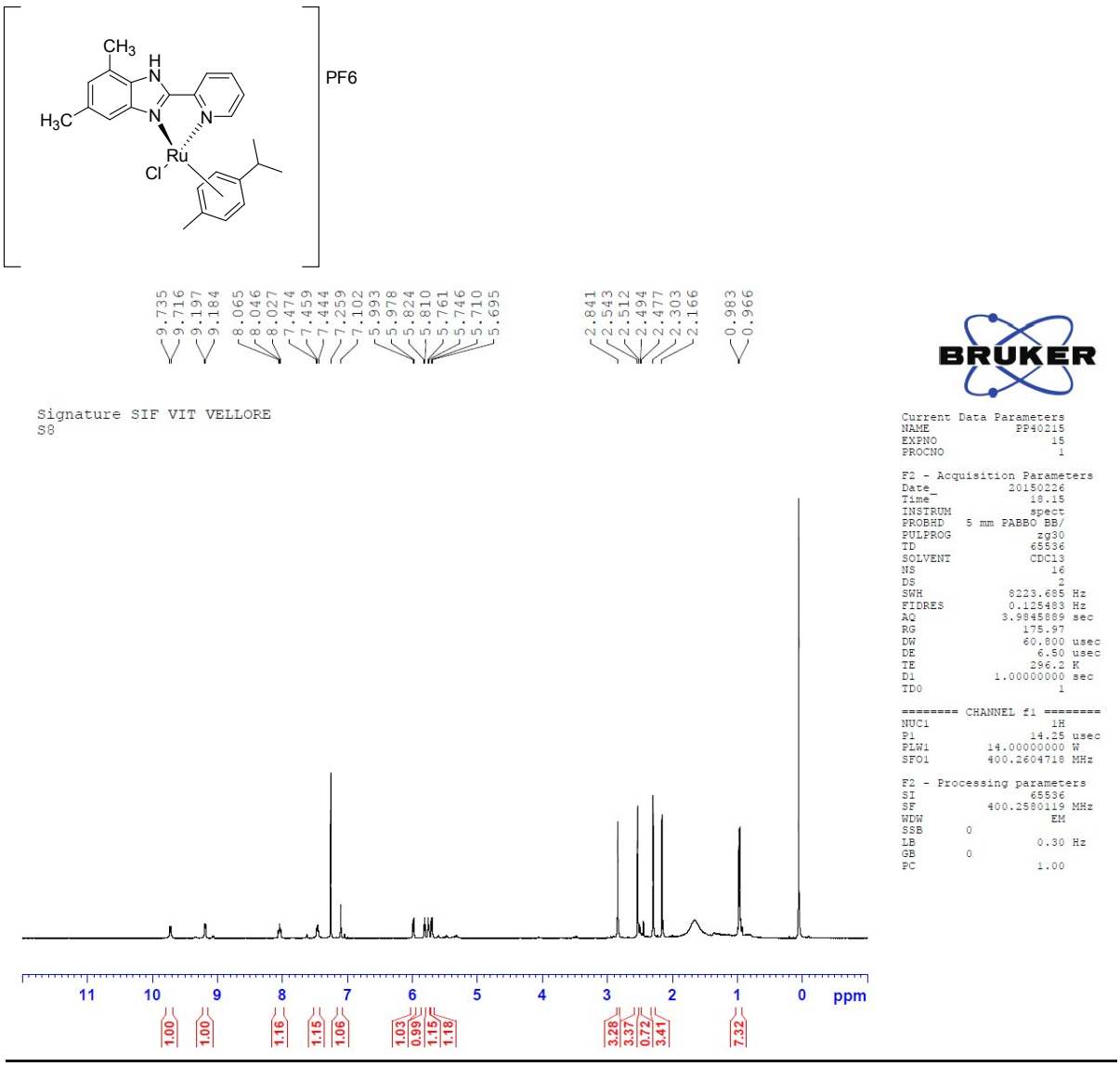



**Figure S19-** $^{1}$H NMR of complex **4e**

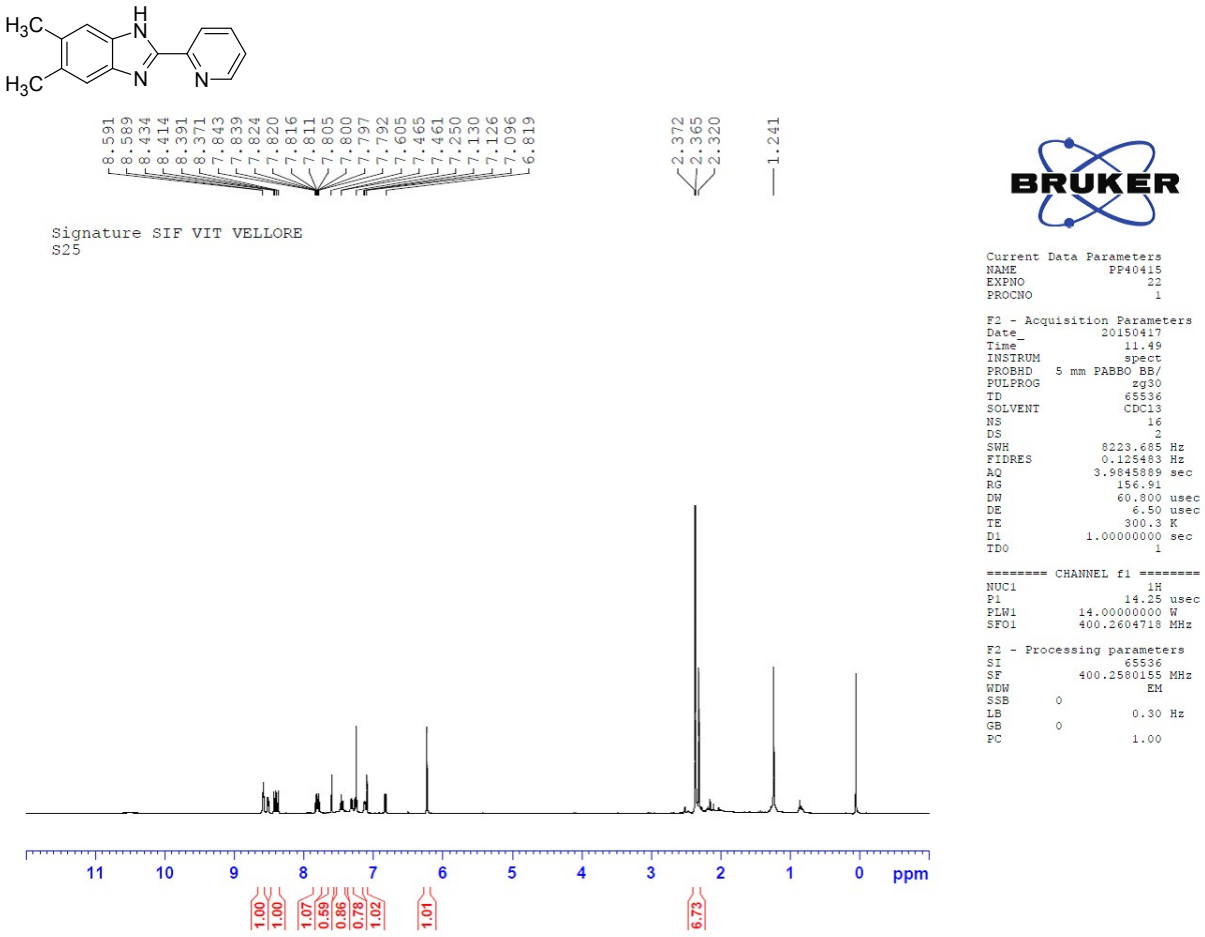



**Figure S20-** $^{1}$H NMR of ligand **3f**

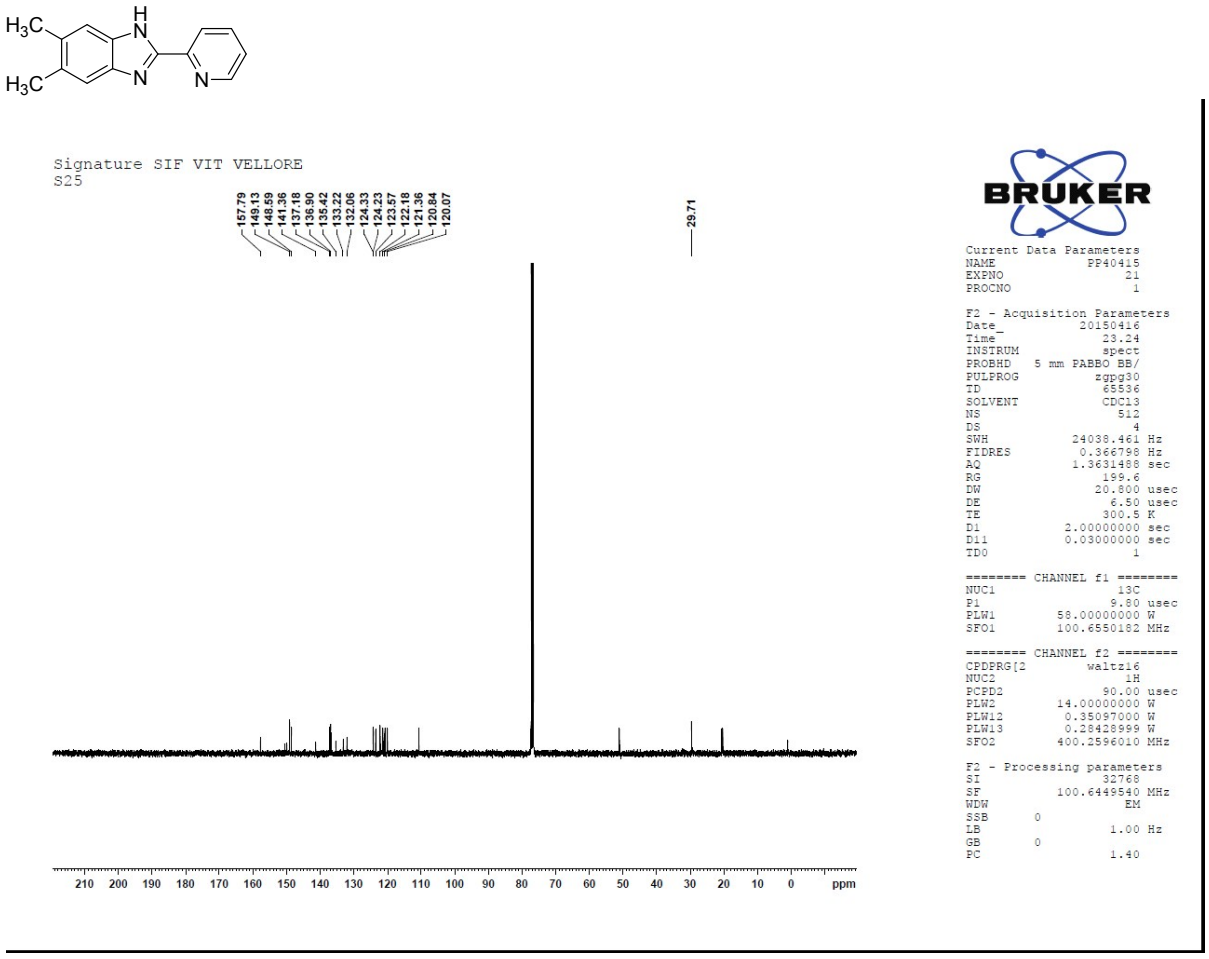
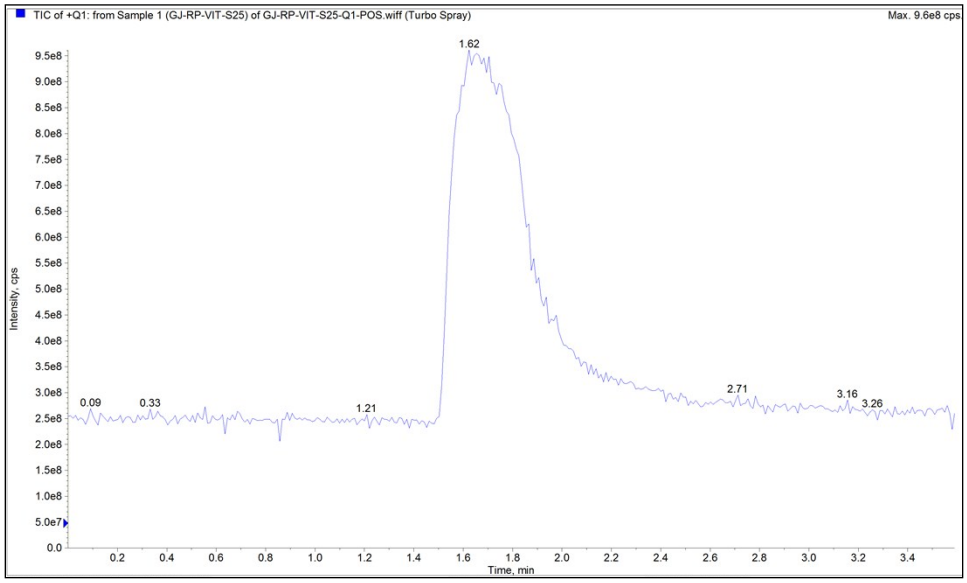



**Figure S21-** $^{13}$C NMR of ligand **3f**

TOTAL ION CHROMATOGRAMS (TIC)




1) MOLECULAR ION (Q1)

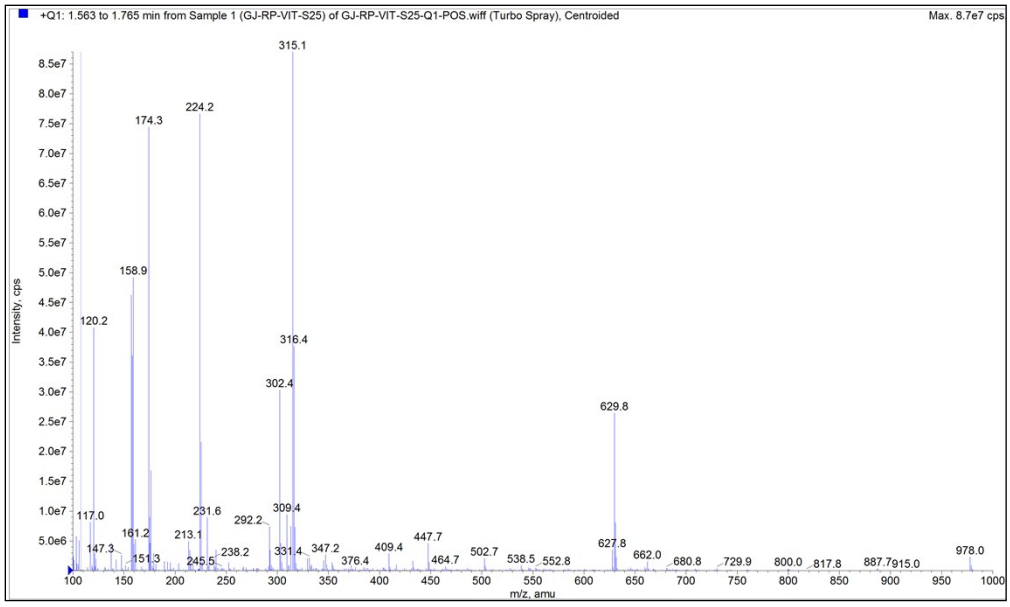



**Figure S22-** MS data for compound **3f**

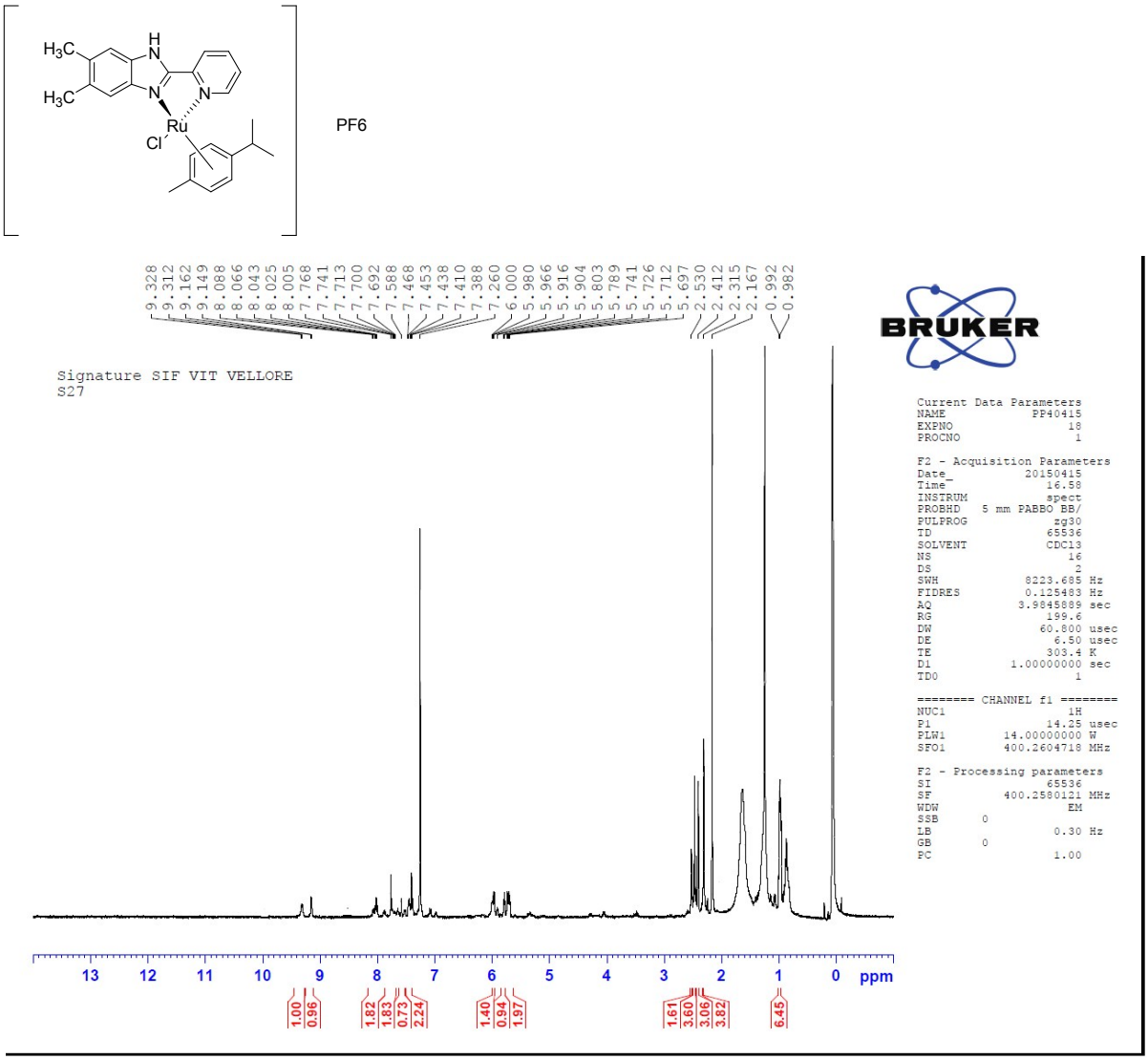
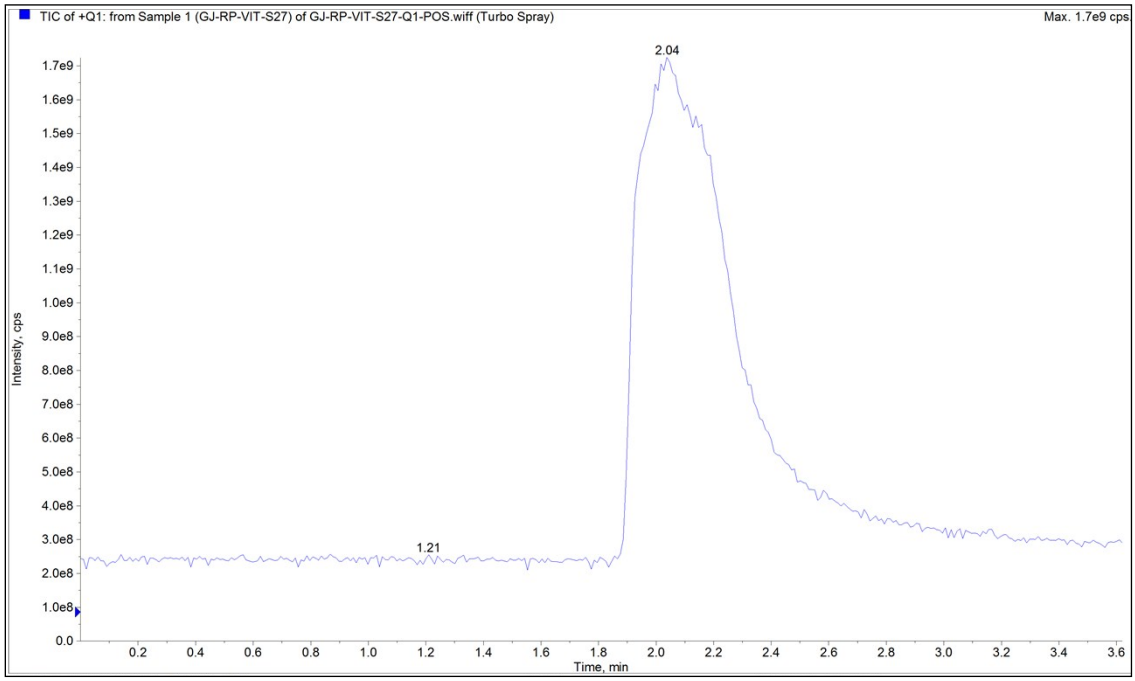



**Figure S23-** $^{1}$H NMR of complex **4f**

TOTAL ION CHROMATOGRAMS (TIC)



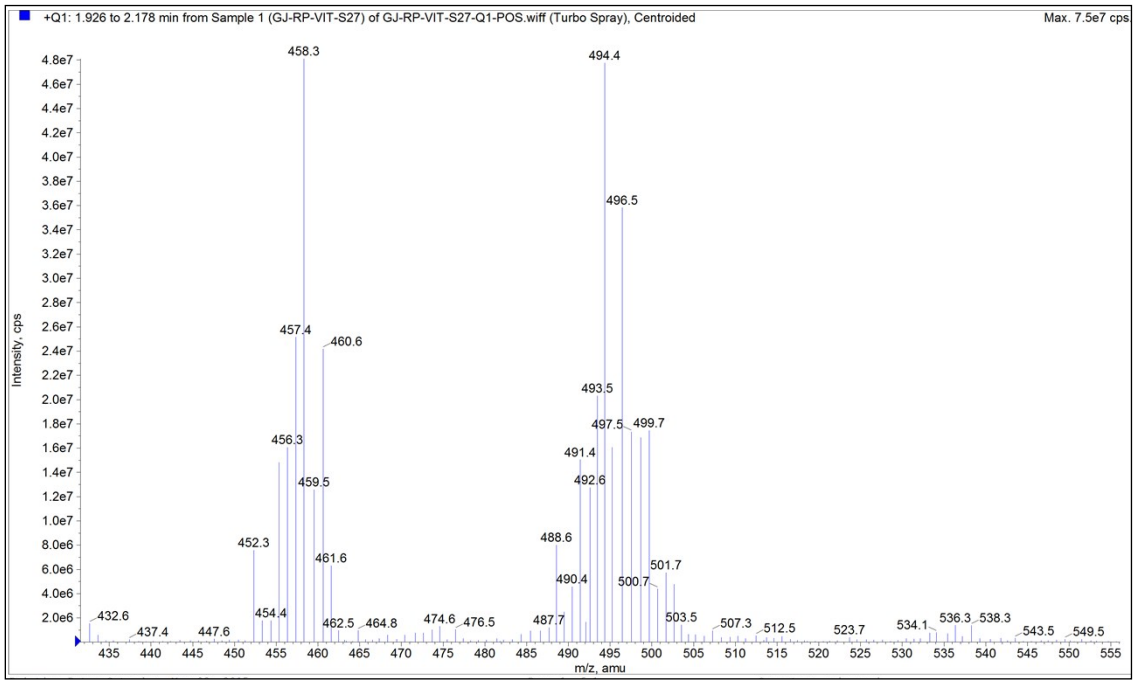




**Figure S24-** MS data for compound **4f**

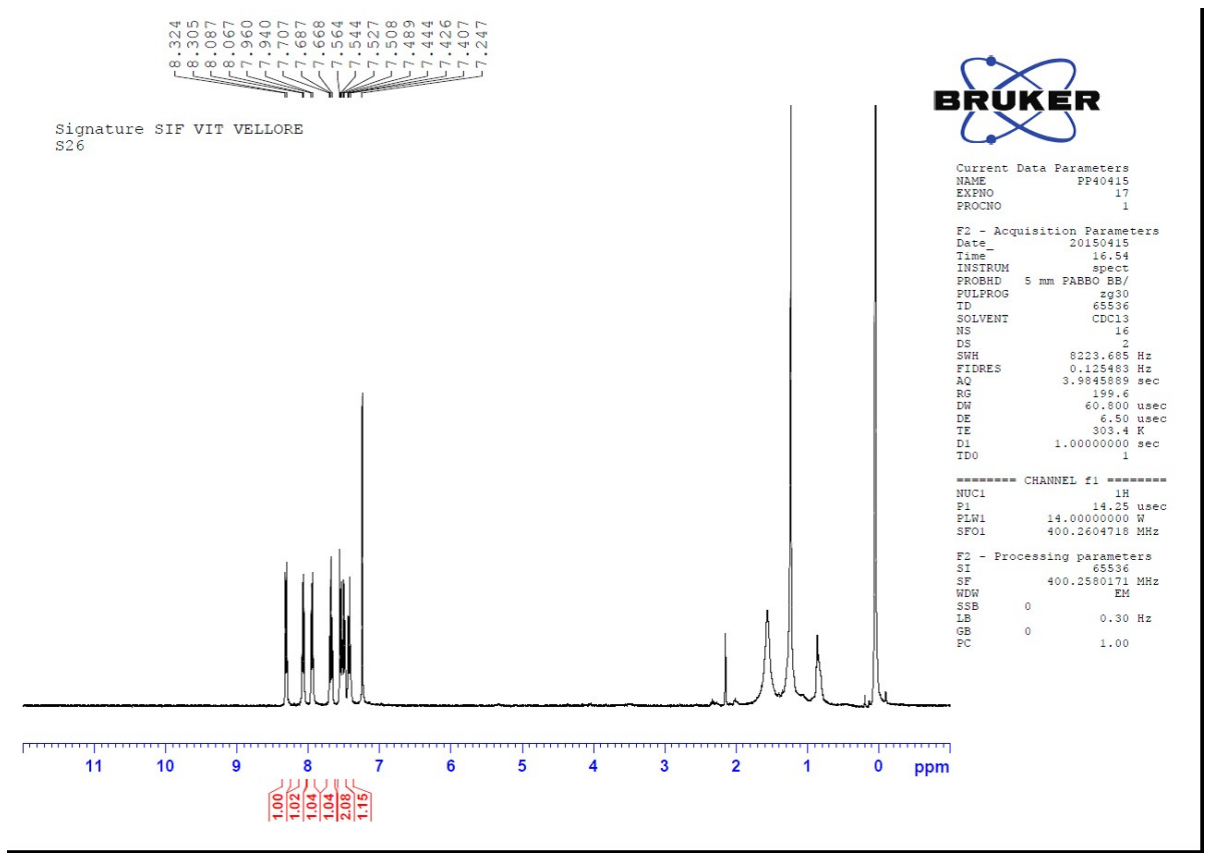
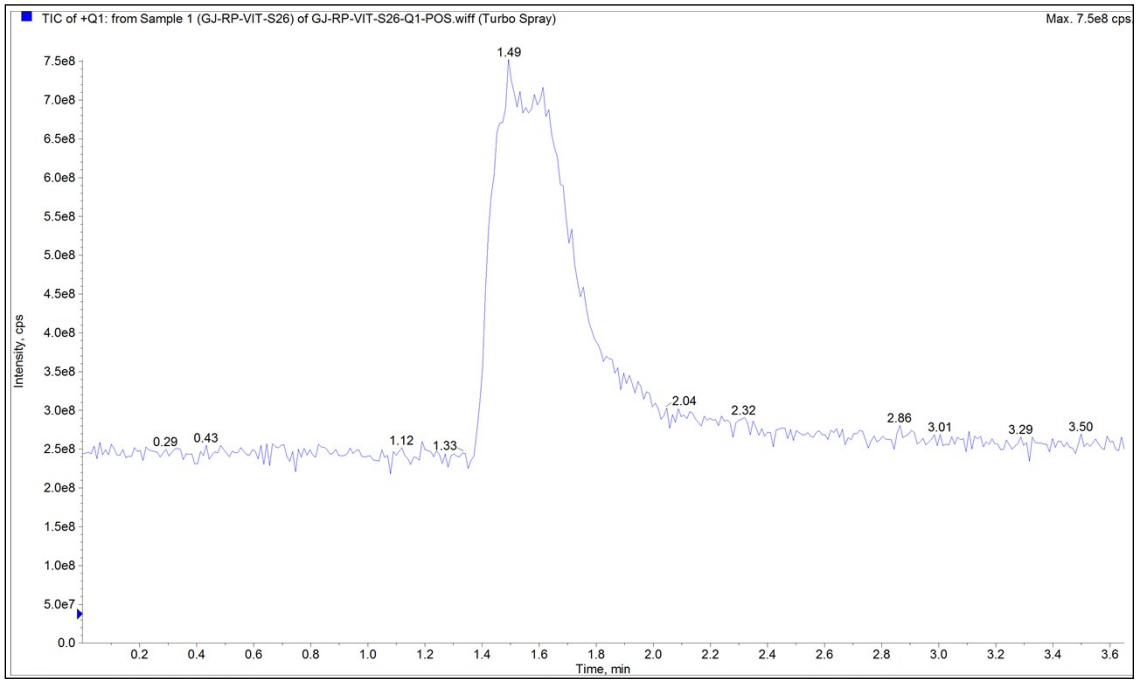
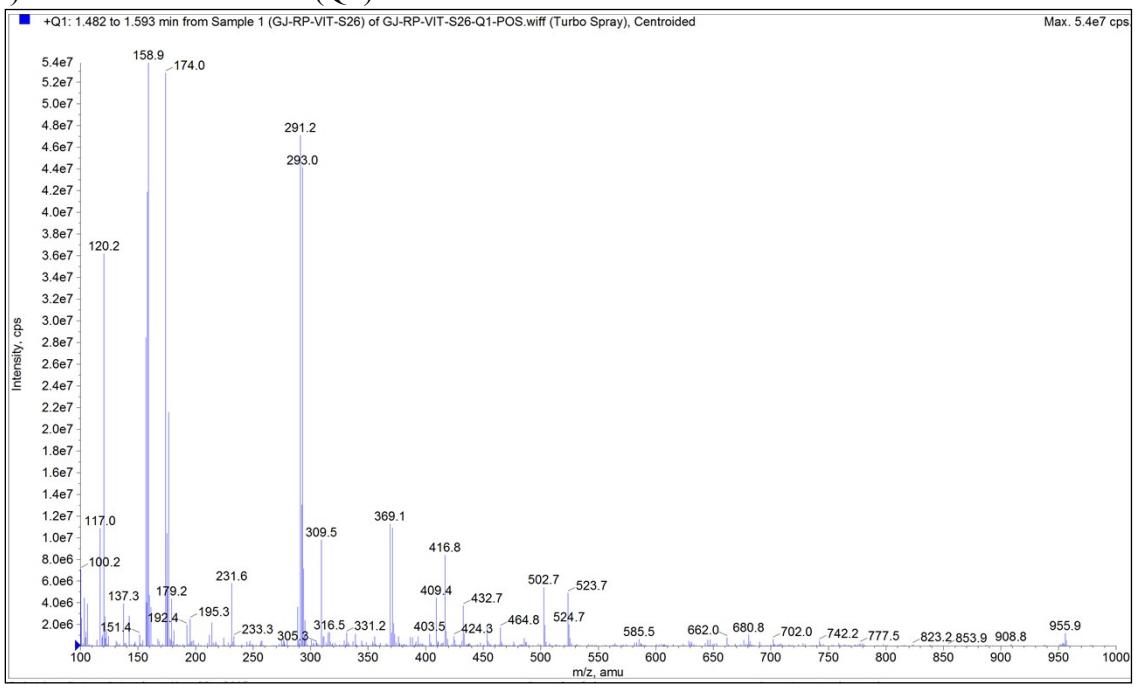



**Figure S25-** $^{1}$H NMR of ligand **3g**

TOTAL ION CHROMATOGRAMS (TIC)




1) MOLECULAR ION (Q1)



2) ZOOM IN VIEW

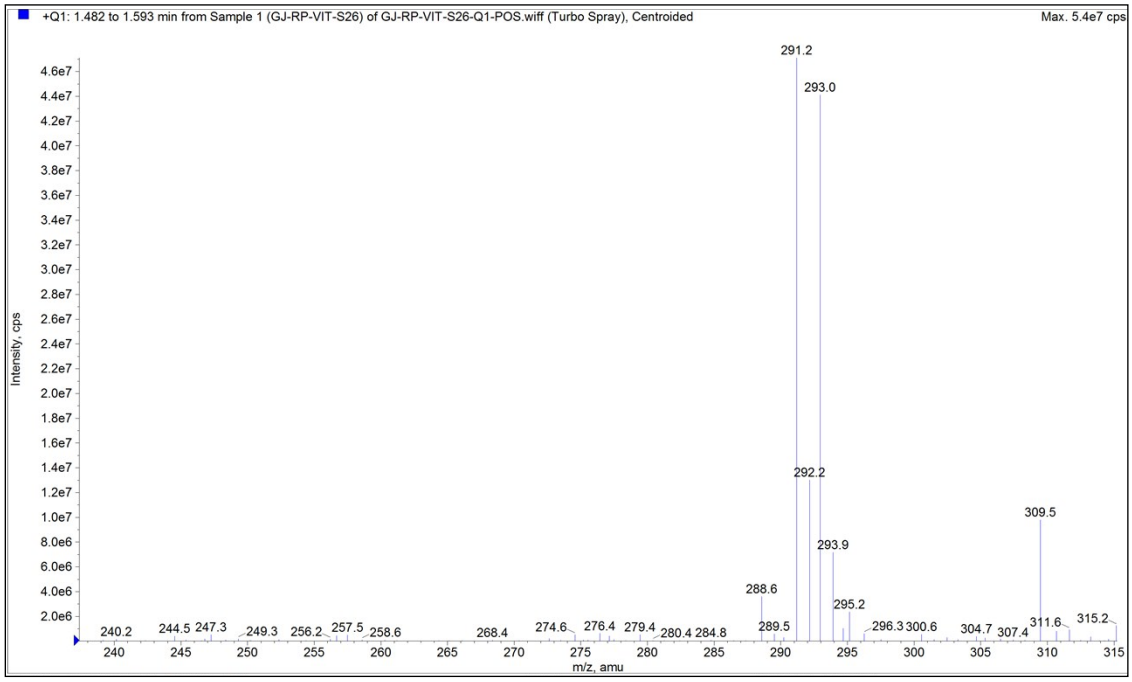



**Figure S26-** MS data for compound **3g**

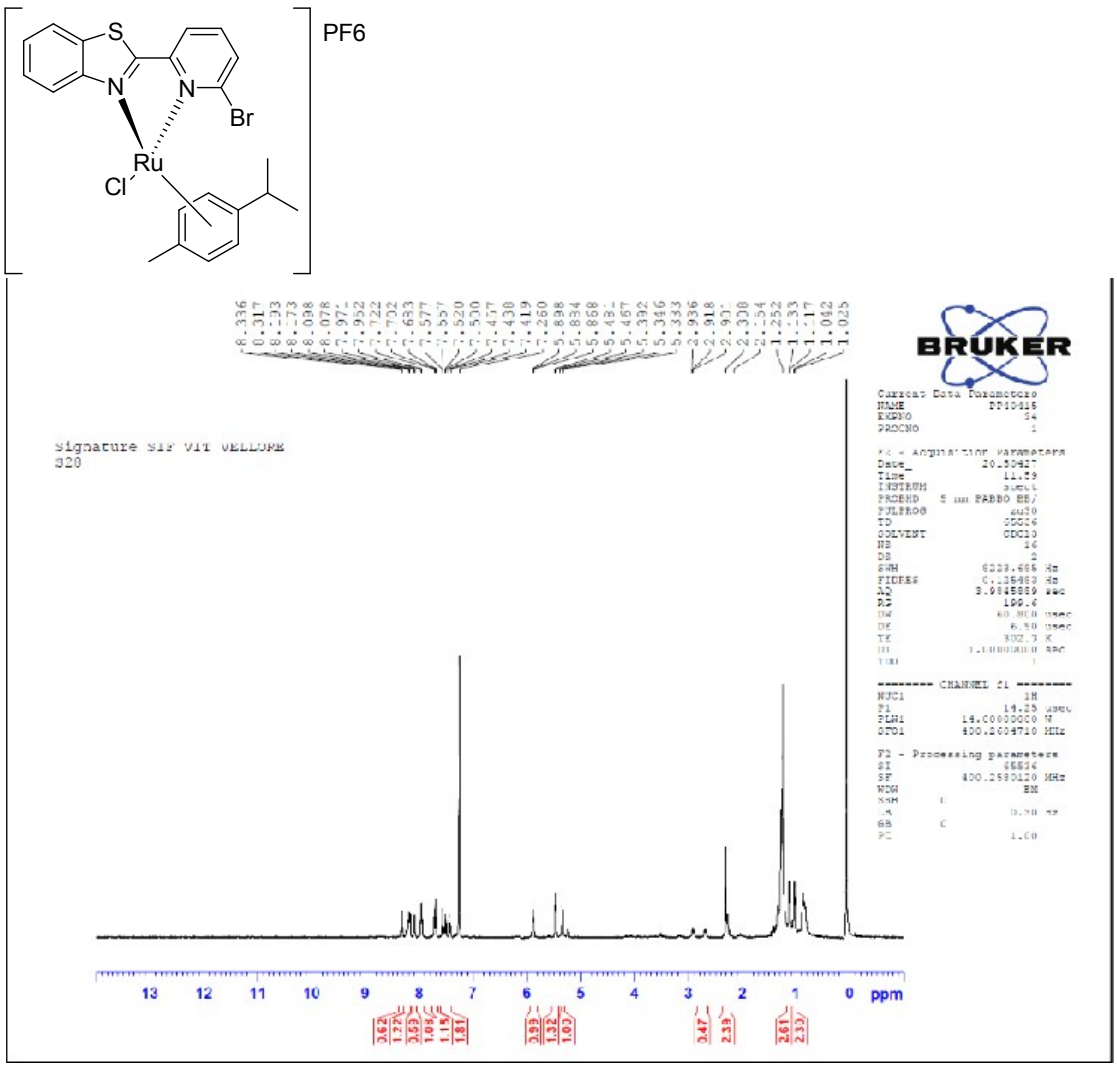



**Figure S27-** $^{1}$H NMR of complex **4g**

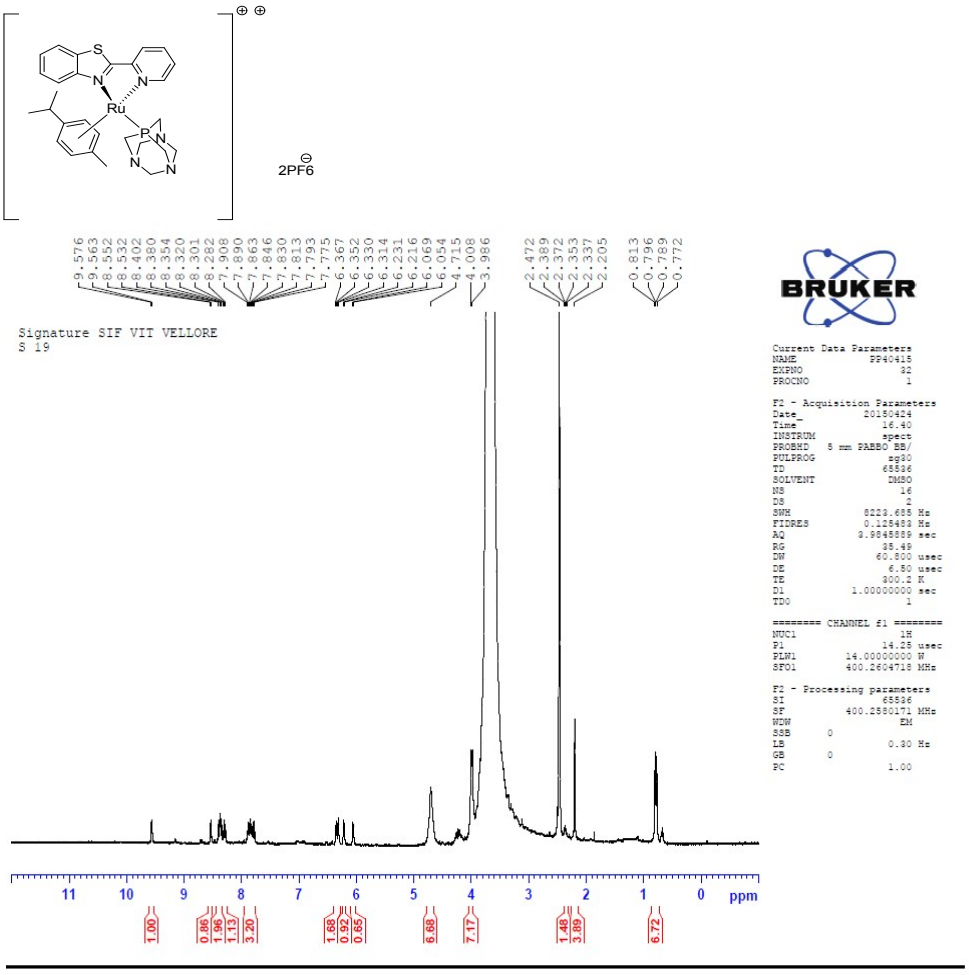



**Figure S28-** $^{1}$H NMR of complex **5a**

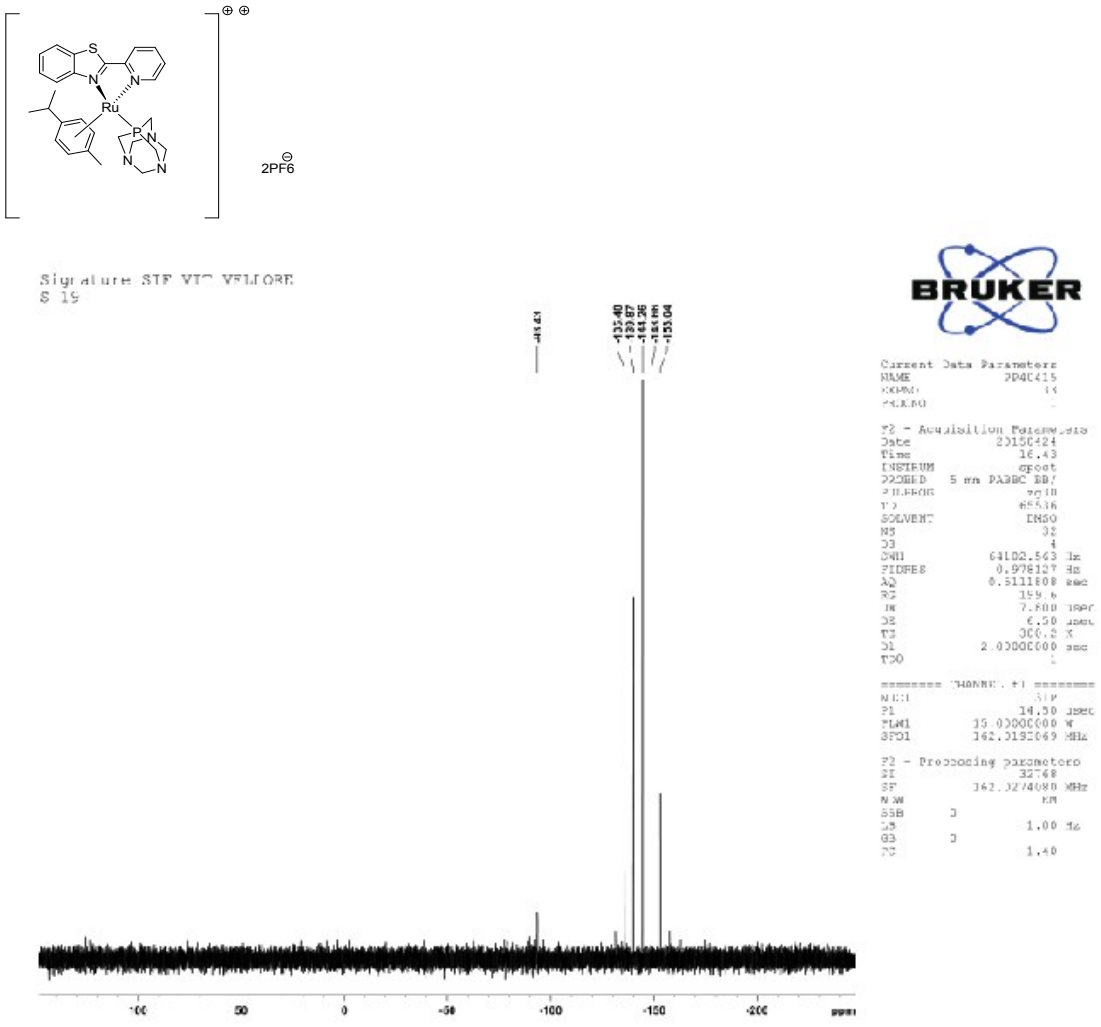
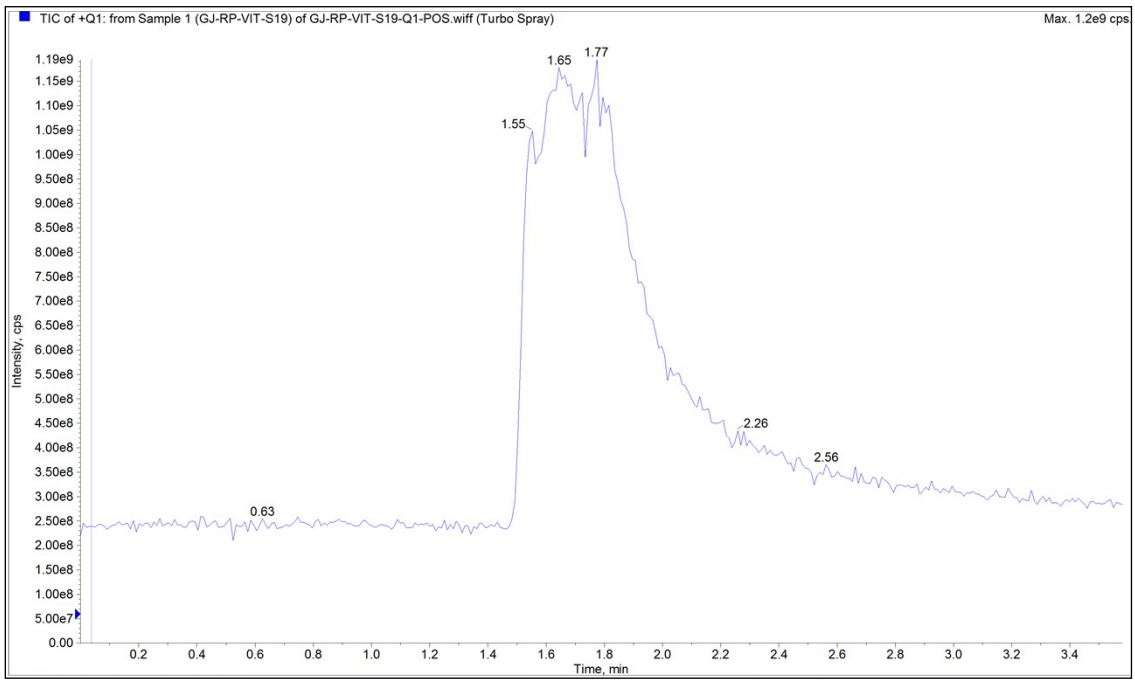



**Figure S29-** $^{31}$P NMR of complex **[(η6-*p*-cymene)RuPTA{2-(pyridin-2-yl)benzo[d]thiazole}]·2PF$_6$ (5a)**

TOTAL ION CHROMATOGRAMS (TIC)



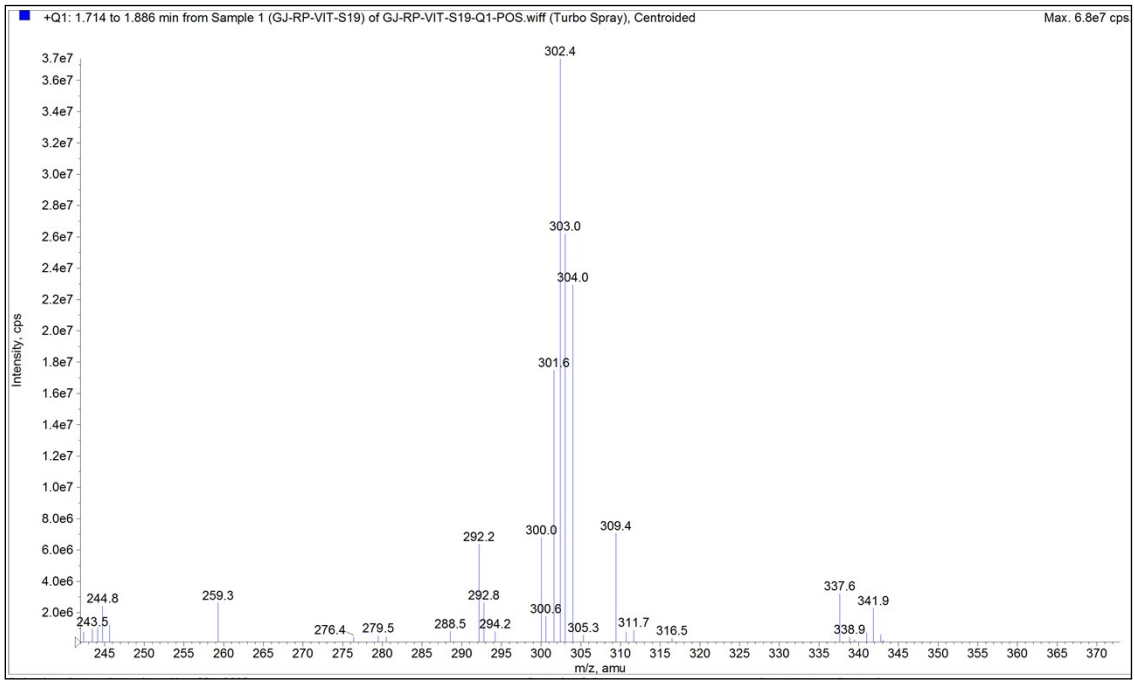




**Figure S30-** MS data for compound **5a**

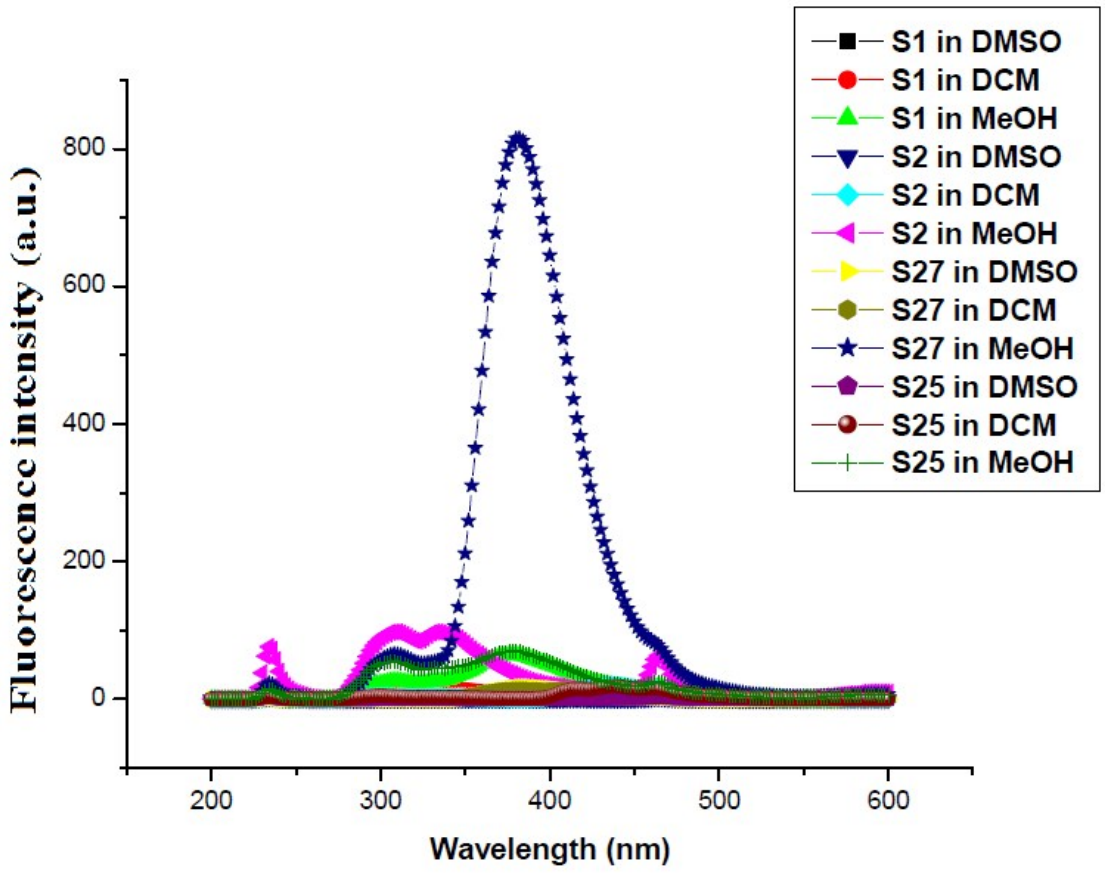



**Figure S31-** Fluorescence spectra of compound **3a (S1)**, **4a (S2)**, **3g (S25)**, **4g (S27)**

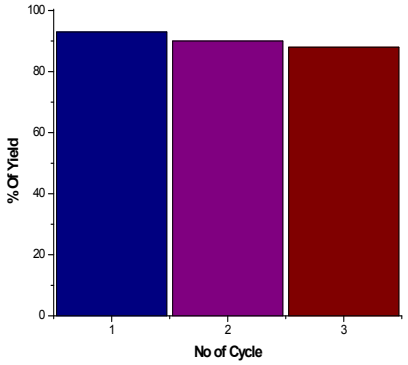



**Figure S32** Reusability of Amberlite IR-120 resin for the synthesis of complex **4a**

***In vitro* cytotoxic activities (MTT assay):** *In vitro* cytotoxicity was determined using the standard MTT assay. [1] The MTT proliferation assay is based on the reduction of the yellow MTT tetrazolium salt (3-[4,5-dimethylthiazol-2-yl]-2,5diphenyltetrazolium bromide) by mitochondrial dehydrogenases to form a blue MTT formazan in viable cells. Test compounds (**4a-g**, **5a**) were practiced prior to the experiment by dissolving in 0.1% DMSO and then serial dilution with medium. Four different types of cancer cell lines i.e. MCF-7 (breast cancer cell line) and human Epitheloid Cervix Carcinoma (HeLa), A2780 and one normal fibroblast MRC-5 were used in the assay. Approximately $4 \times 10^3$ cells per well for A2780 and and $1 \times 10^4$ cells per well for either MCF-7 and MRC-5 were cultured in 100 µL of a growth medium in 96-well plates and incubated at 37 °C under a 5% $CO_2$ atmosphere. The cells were then treated with different concentrations of the drugs (1-100 µM) in the volume of 100 µM /well. Cisplatin has been used as a standard positive control drug. Cells in the control wells accepted the same volume of medium containing 0.1% DMSO. After 24 h, the medium was discarded and cell cultures were incubated with 100 ml MTT reagent (1 mg/ml) for 5 h at 37$^o$ C. Then the suspension was placed on microvibrator for 10 min and subsequently the absorbance was recorded by the ELISA reader at $\lambda$ = 620 nm. The experiment was also performed in triplicate. The data were expressed as the growth inhibition percentage calculated according to the equation: % growth inhibition = 100 − [(AD × 100)/AB], where AD is the measured absorbance in wells containing samples and AB is the absorbance measured for blank wells (cells with a medium and a vehicle). Human cancer cell lines, MCF-7 and HeLa cells were cultured in MEM medium supplemented with 10% FBS, 1% glutamine and 50 mM/ml gentamicin sulphate in a $CO_2$ incubator in a humidified atmosphere of 5% $CO_2$ and 95% air. The growth media RPMI 1640 with 10% fetal bovine serum (FBS) and 2 mM Lglutamine in a 95% air, 5% CO2 atmosphere for A2780 cells, minimun essential medium eagle (EMEM) with 10% FBS in 95% air, 5% CO2 atmosphere for MRC-5 has been used.

**References**

1 (a) T. Mossman, *J. Immunol. Methods*, 1983, **65**, 55-63.; (b) S. Saeed, N. Rashid, P. G. Jones, M. Ali and R. Hussain, *Eur. J. Med. Chem.*, 2010, **45**, 1323-1331.