Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2019

Supporting Information

Direct Synthesis of 2,4,5- Trisubstituted Imidazoles From Primary Alcohols By Diruthenium(II) Catalysts under aerobic conditions

Sundar Saranya,[a] and Rengan Ramesh*[a]

[a]Centre for Organometallic Chemistry, School of Chemistry, Bharathidasan University,

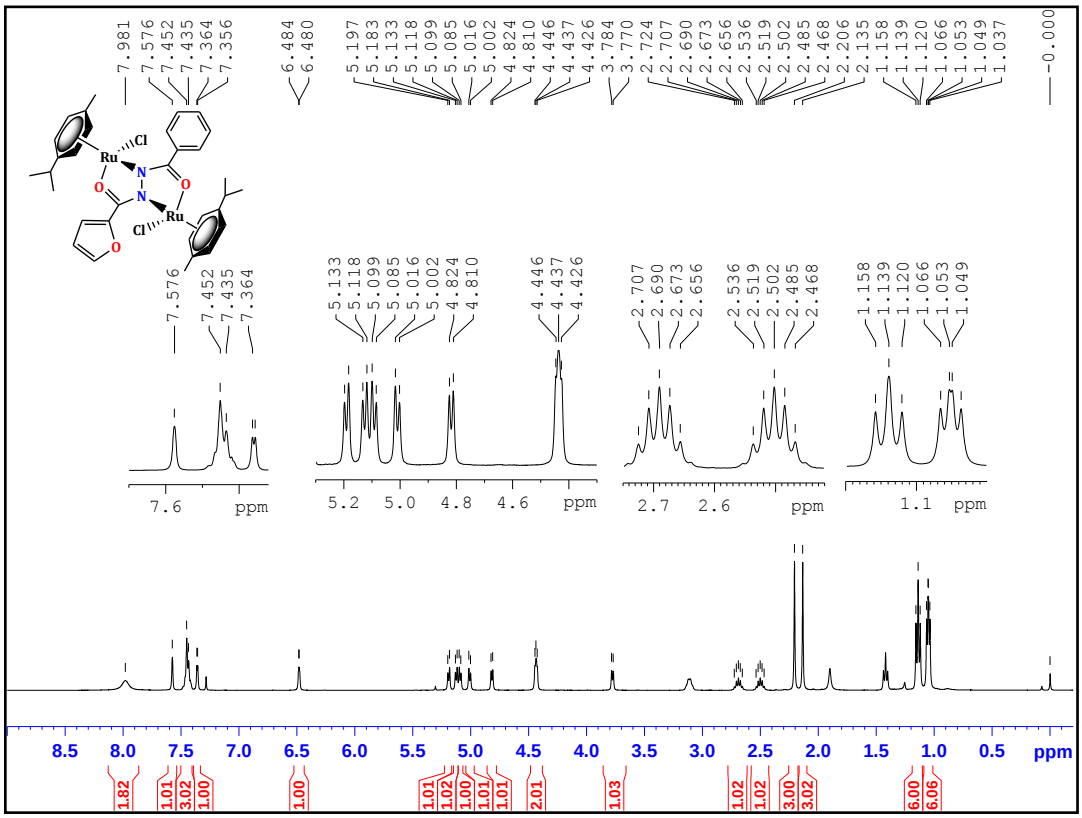
Tiruchirappalli 620 024, Tamil Nadu, India

CONTENTS:

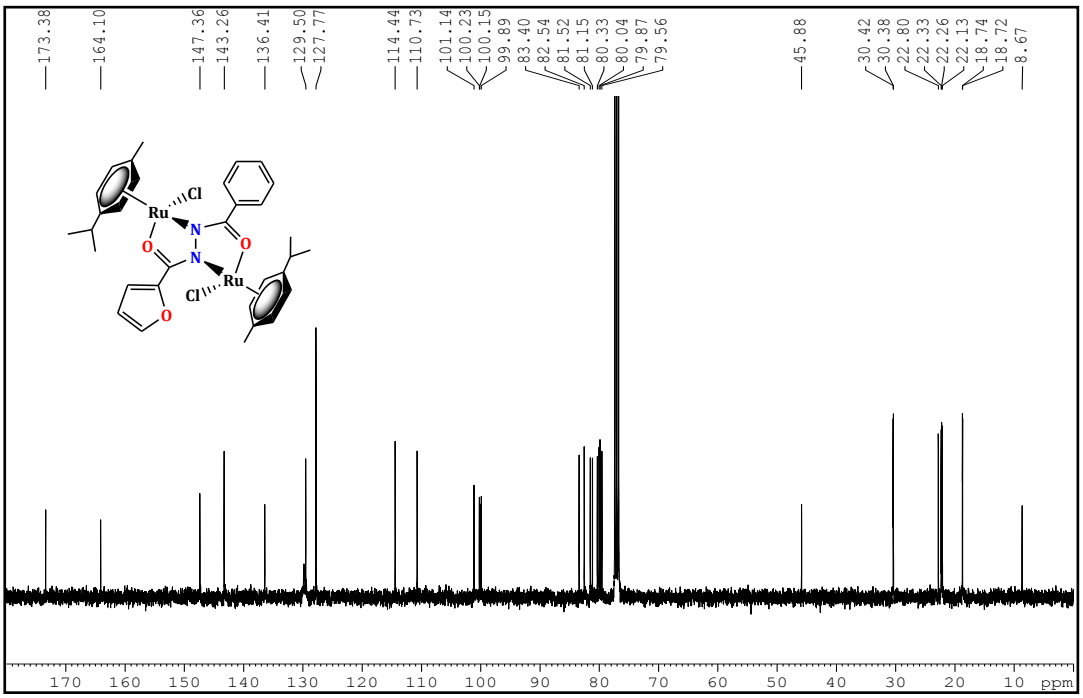
1. General Information

N'-benzoylfuran-2-carbohydrazide ligand was prepared according to the literature procedure.Unless otherwise noted, all reactions were performed under an atmosphere of air. All solvents were reagent grade or better. Deuterated solvents were used as received. C, H, N and S analyses were carried out with a Vario EL III CHNS elemental analyser. IR spectra were recorded on a JASCO 400 plus spectrometer. Electronic spectra in CH_2Cl_2 solution were recorded with a CARY 300 Bio UV- visible Varian spectrometer. ^{1}H and ^{13}C NMR spectra were recorded at 400 and 100 MHz, respectively, using Bruker Avance-400 NMR spectrometers with $CDCl_3$ and DMSO-d_6 as solvents and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in units (ppm) by assigning TMS resonance as 0.00 ppm. Abbreviations used in the NMR follow-up experiments: br, broad; s, singlet; d, doublet; t, triplet; m, multiplet. High Resolution Mass spectra were recorded on a Thermo Exactive Orbitrap mass spectrometer using electrospray ionization (ESI) technique.

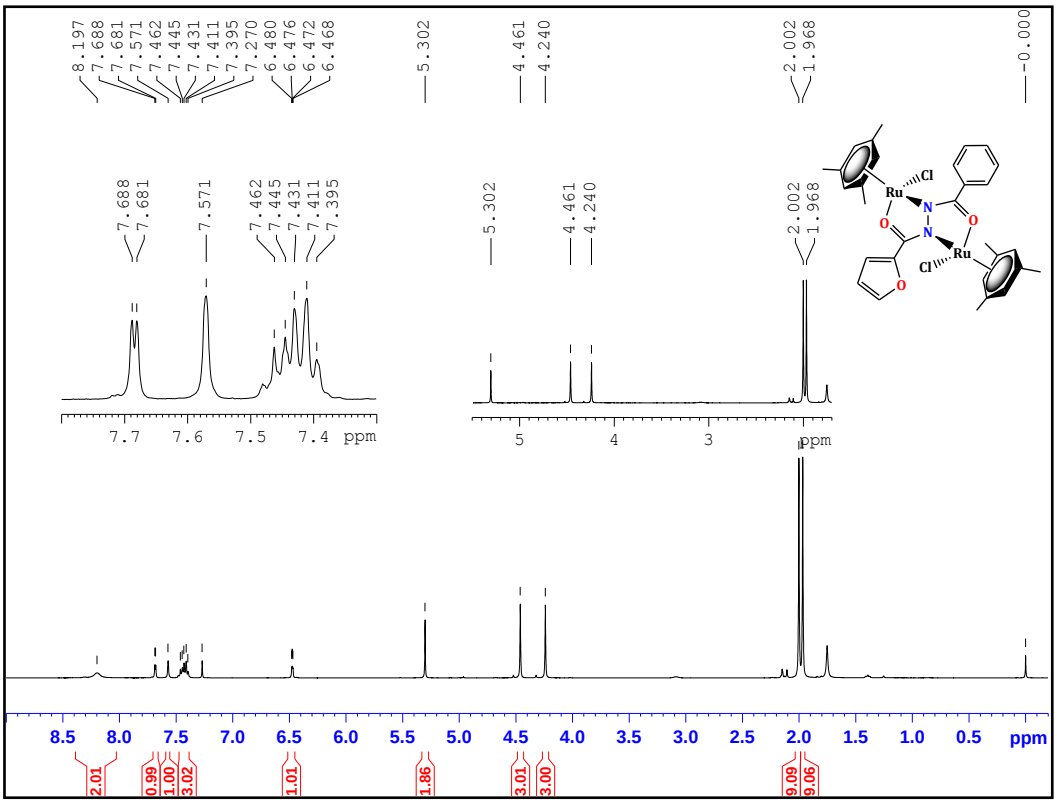
2. ^{1}H NMR and ^{13}C NMR spectrum of complexes 1 and 2



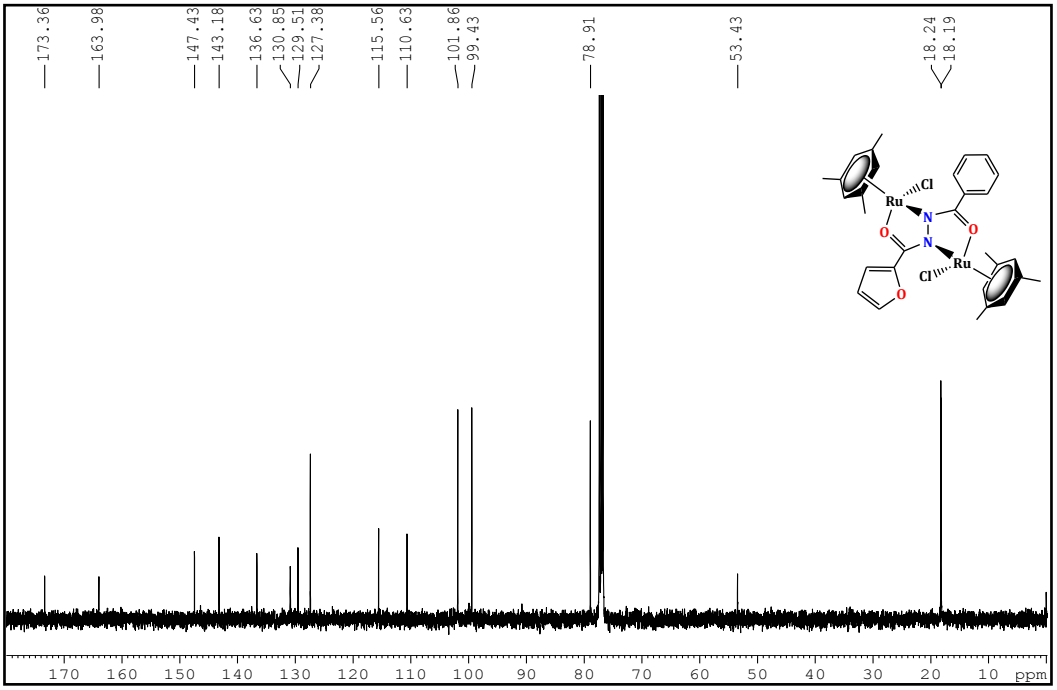
^{1}H NMR spectrum of complex 1



^{13}C NMR spectrum of complex 1

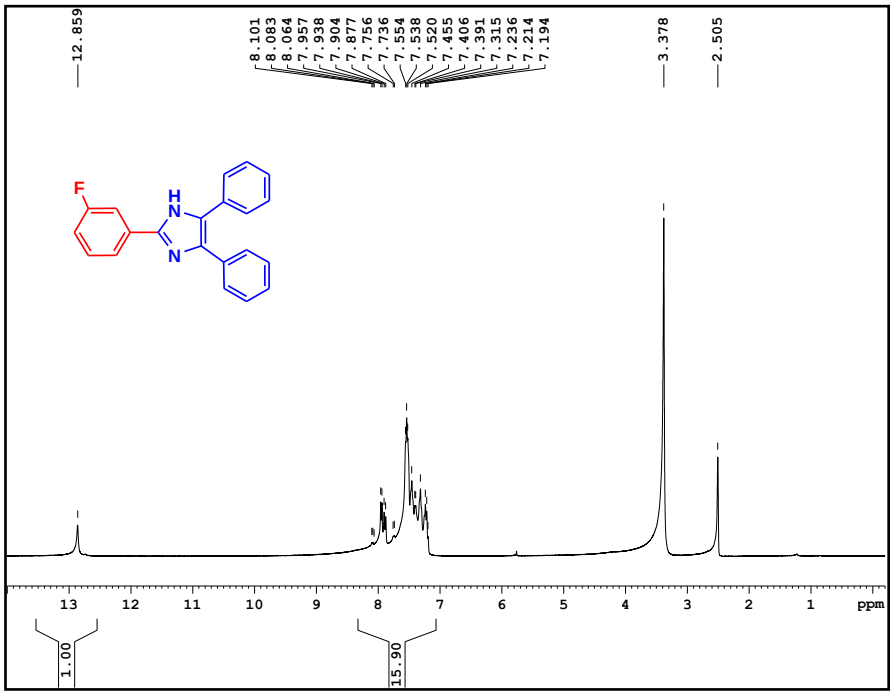


^{1}H NMR spectrum of complex 2

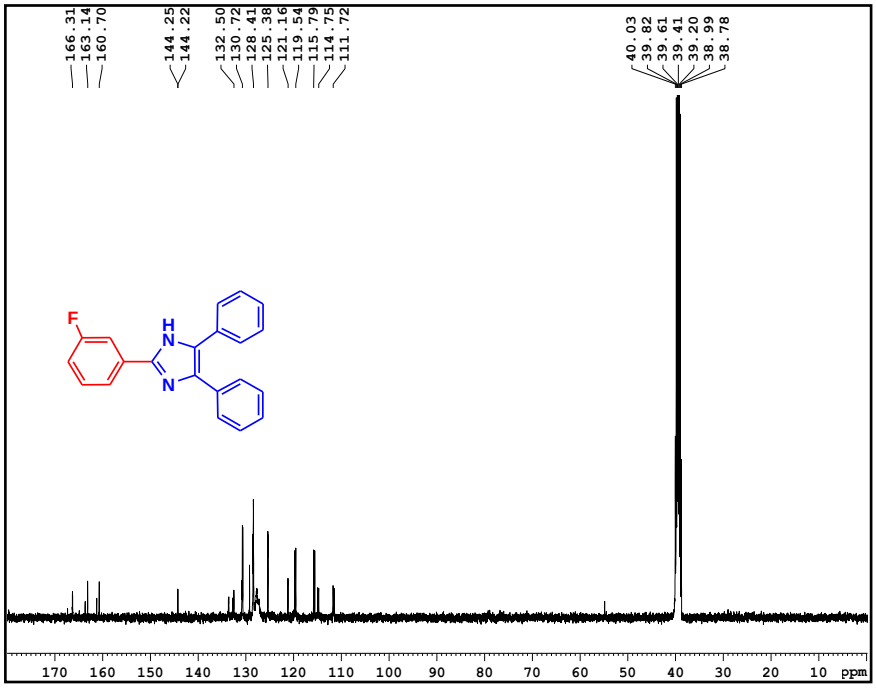


^{13}C NMR spectrum of complex 2

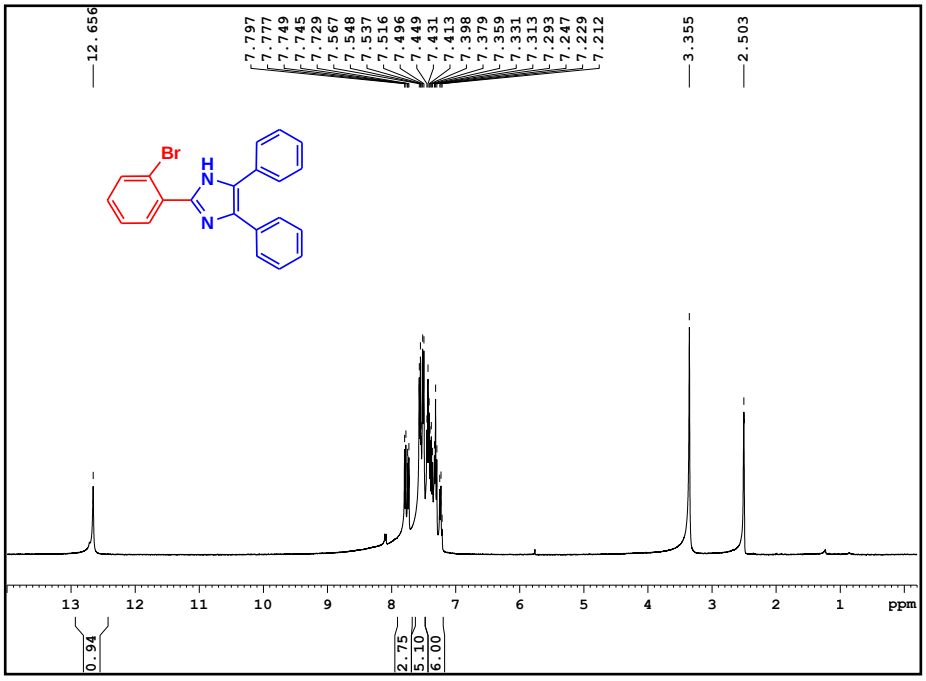
3. ^{1}H NMR and ^{13}C NMR spectrum of representative tri-substituted imidazoles



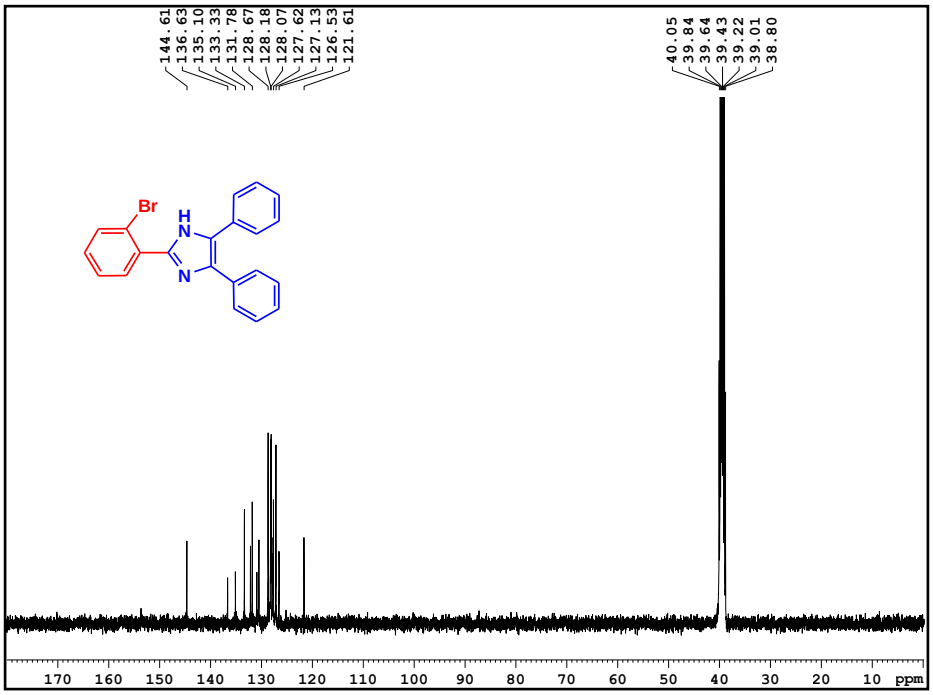
^{1}H NMR (400 MHz, DMSO-*d6*) spectrum of 5g(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



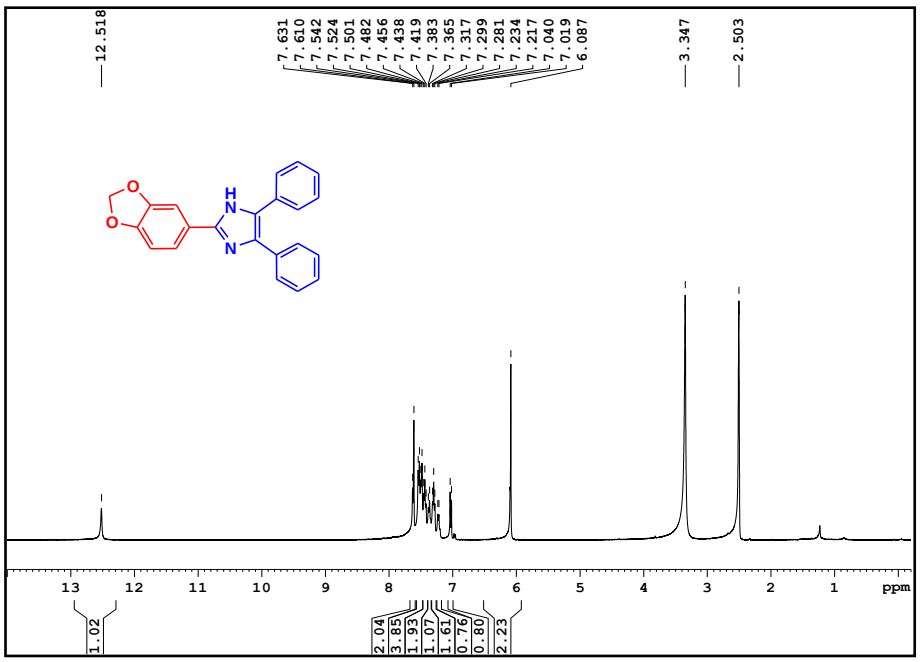
^{13}C NMR (100 MHz, DMSO-*d6*) spectrum of 5g



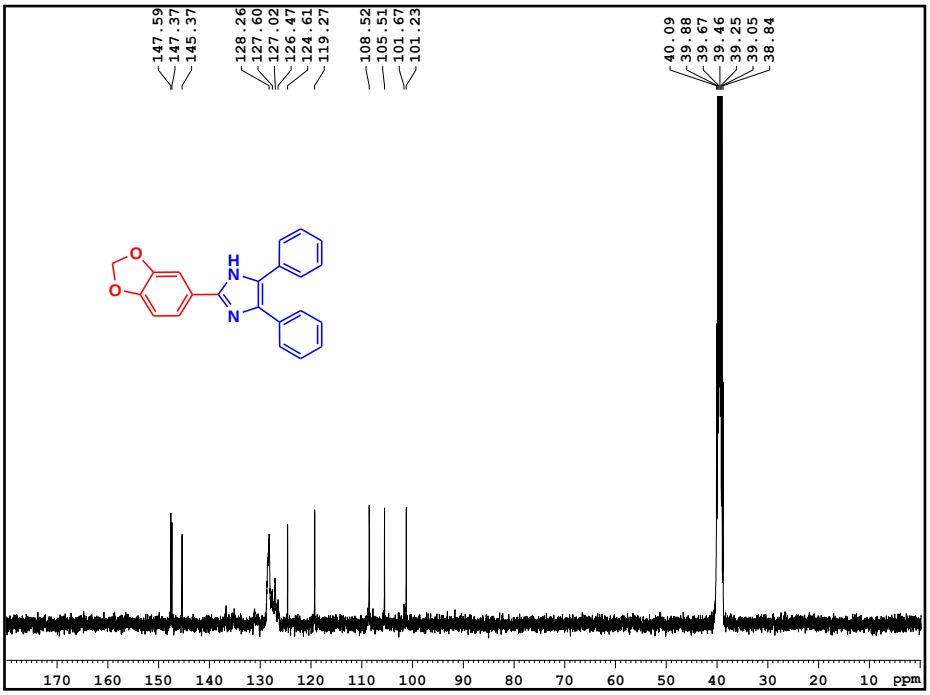
[1]H NMR (400 MHz, DMSO-*d6*) spectrum of 5i(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



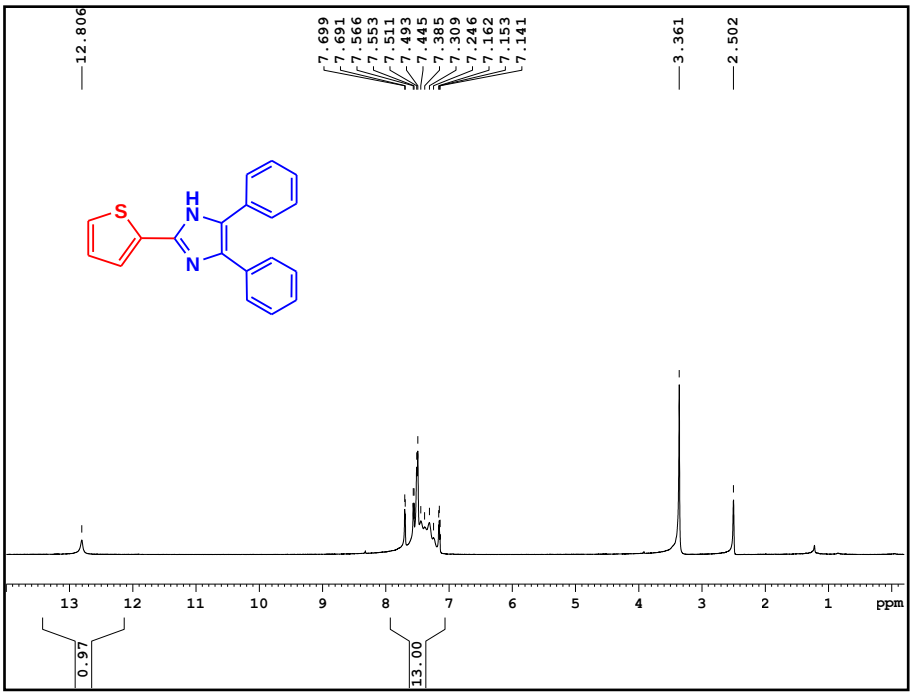
[13]C NMR (100 MHz, DMSO-*d6*) spectrum of 5i



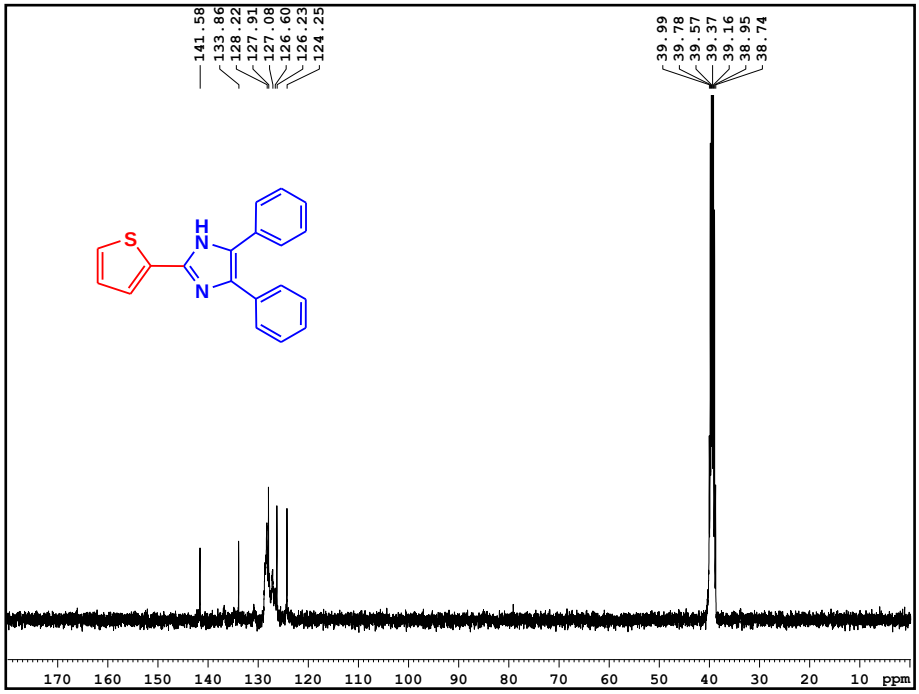
[1]H NMR (400 MHz, DMSO-*d6*) spectrum of 5j(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



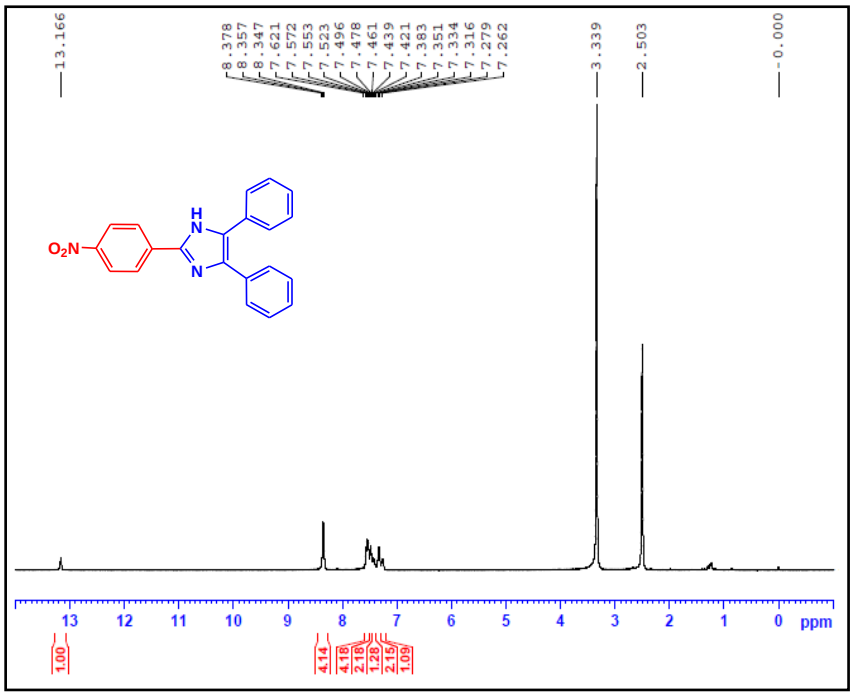
[13]C NMR (100 MHz, DMSO-*d6*) spectrum of 5j



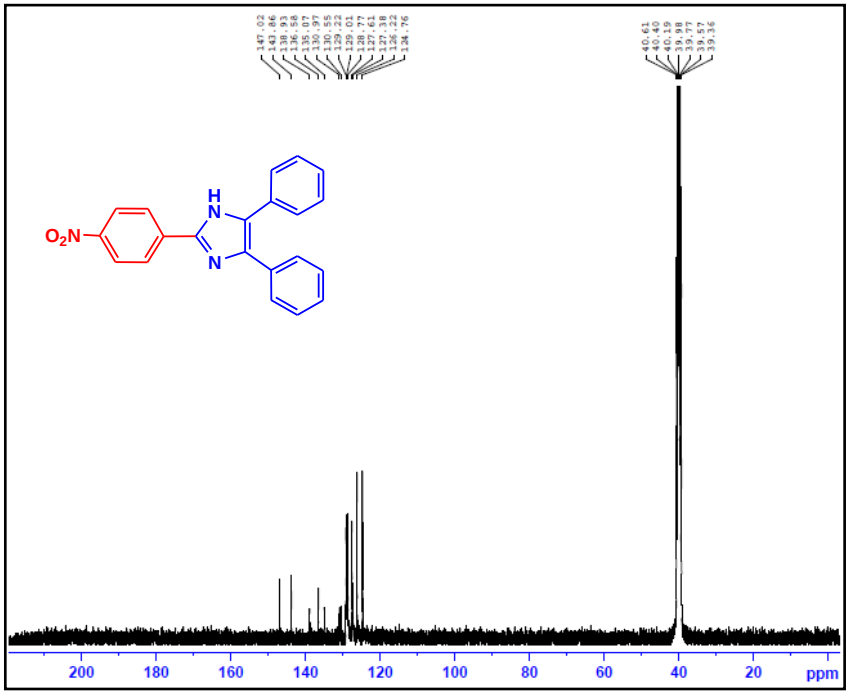
^{1}H NMR (400 MHz, DMSO-*d6*) spectrum of 5k(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



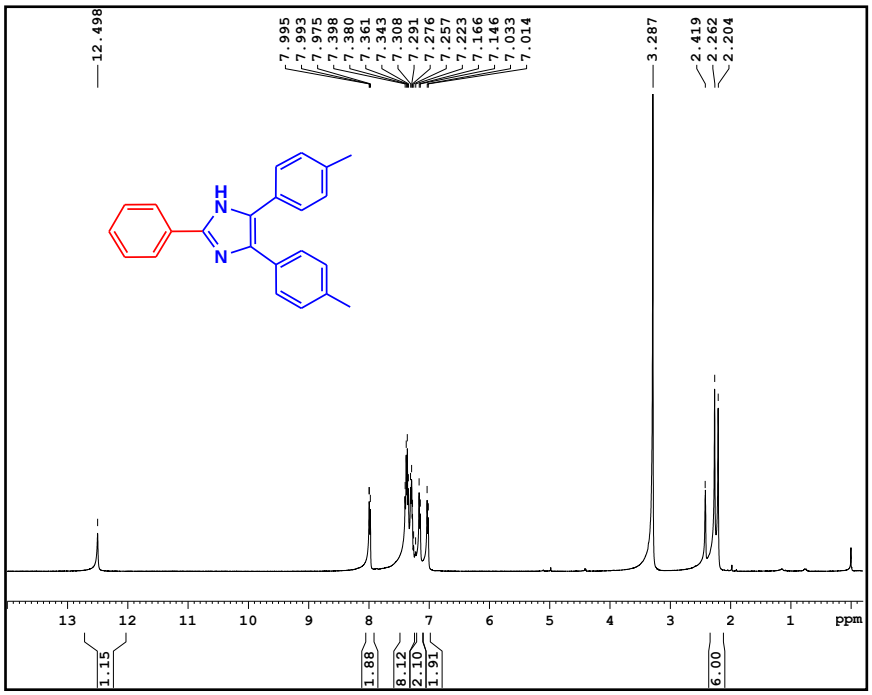
^{13}C NMR (100 MHz, DMSO-*d6*) spectrum of 5k



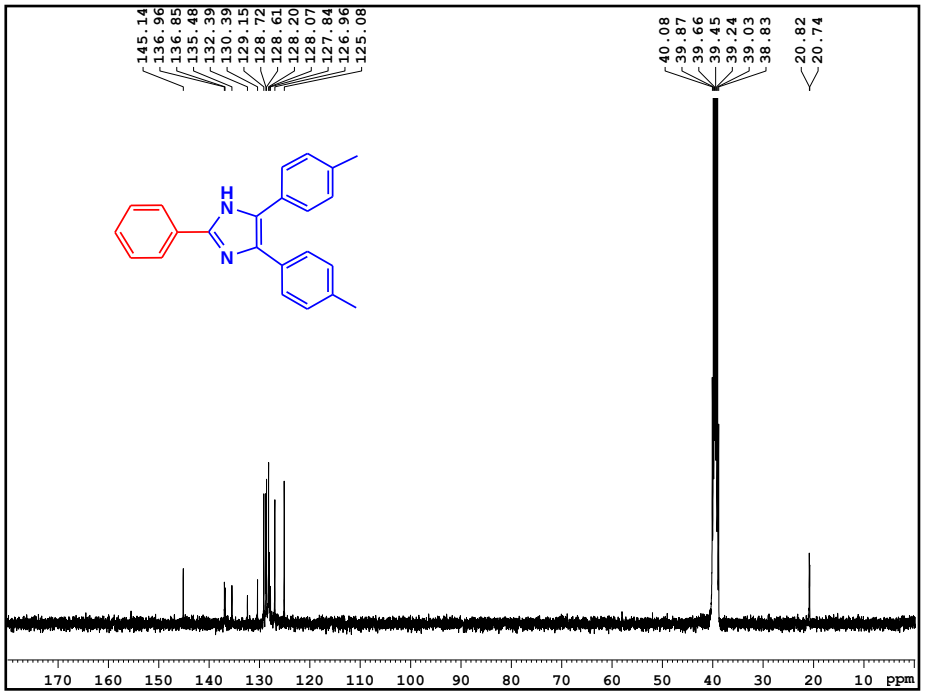
[1]H NMR (400 MHz, DMSO-*d6*) spectrum of 5l (peaks at 3.3 and 2.5 ppm are solvent and water peaks)



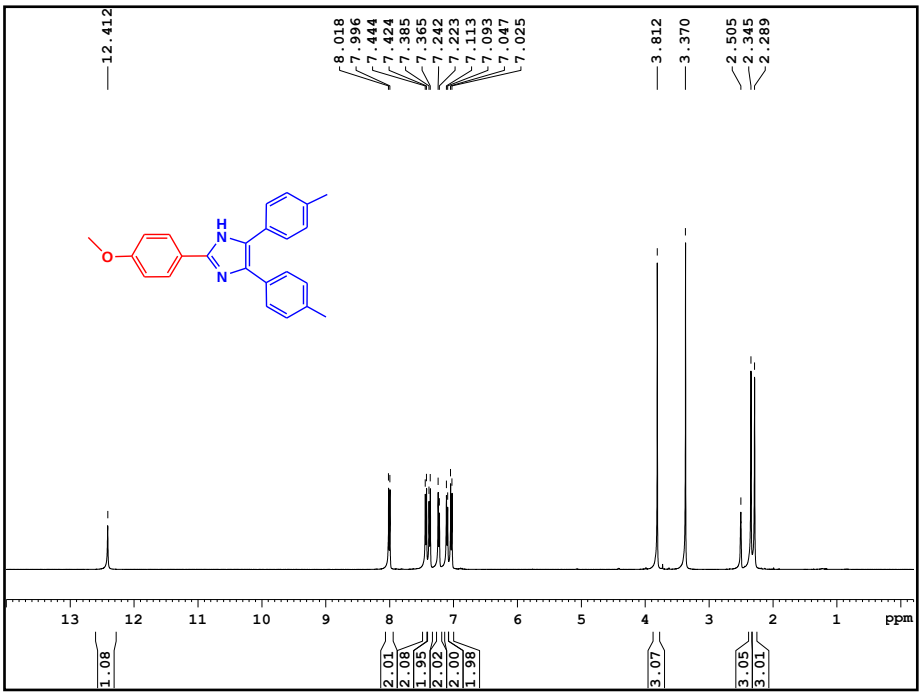
[13]C NMR (100 MHz, DMSO-*d6*) spectrum of 5l



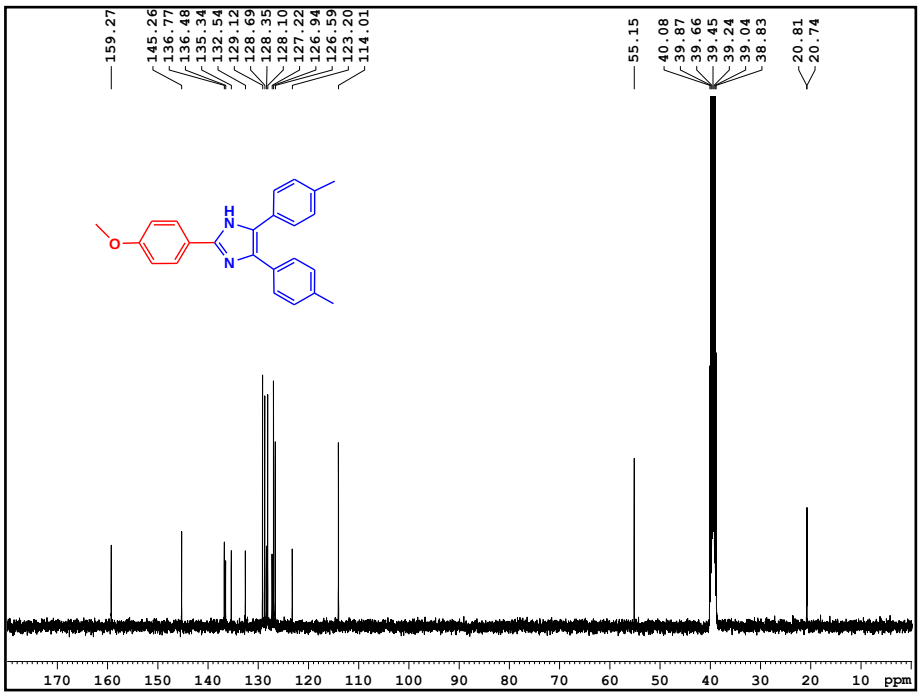
[1]H NMR (400 MHz, DMSO-*d6*) spectrum of 5m(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



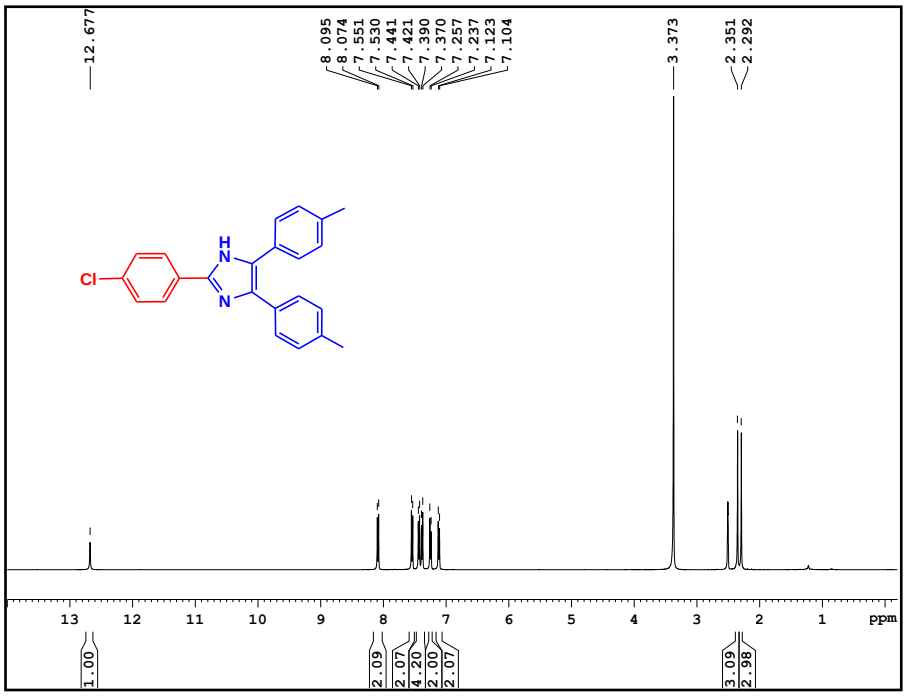
[13]C NMR (100 MHz, DMSO-*d6*) spectrum of 5m



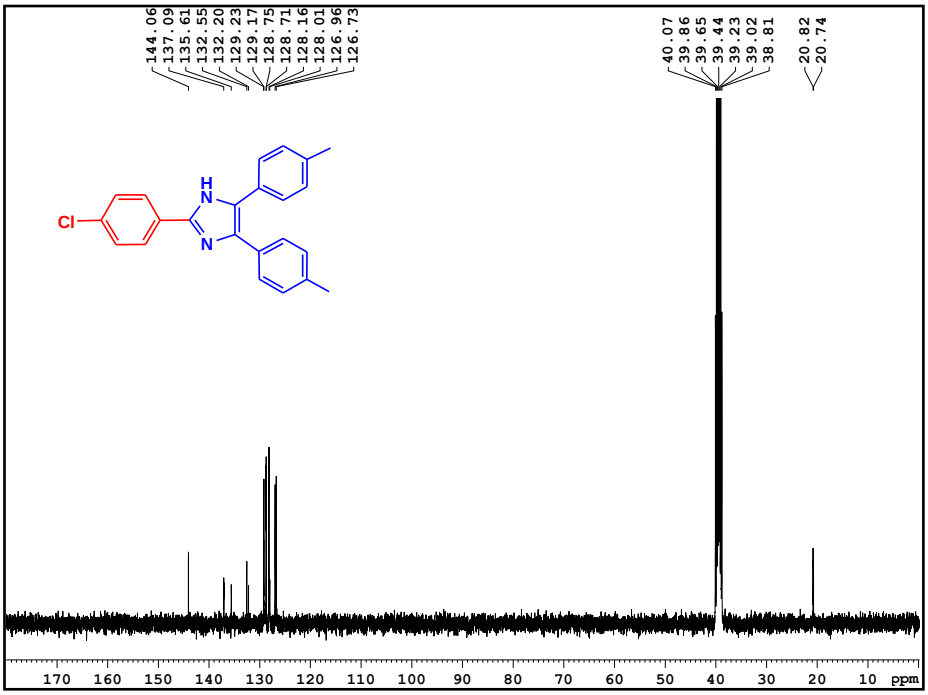
[1]H NMR (400 MHz, DMSO-*d6*) spectrum of 5n(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



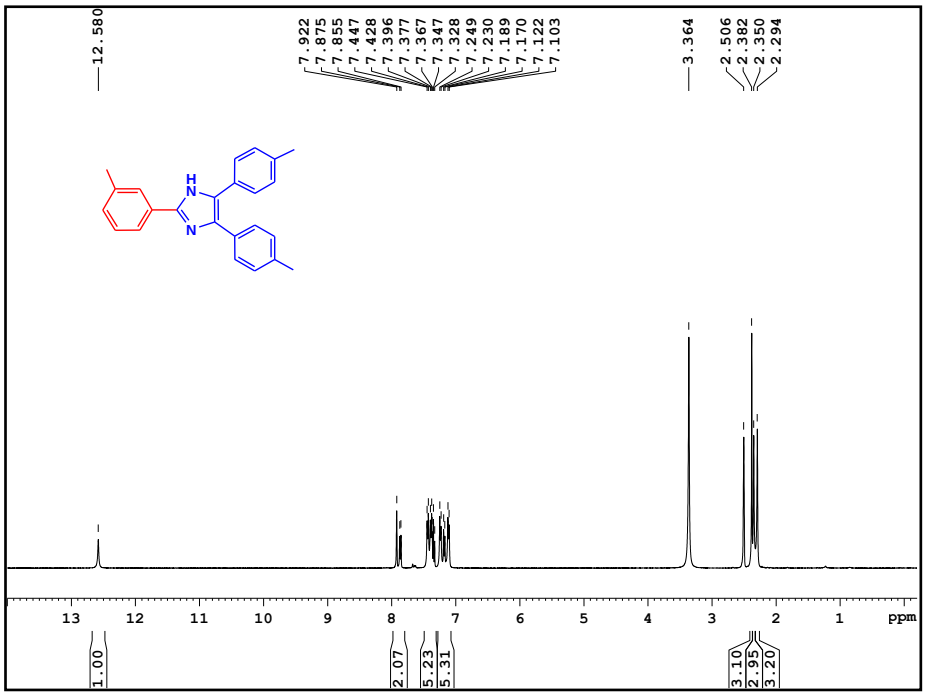
[13]C NMR (100 MHz, DMSO-*d6*) spectrum of 5n



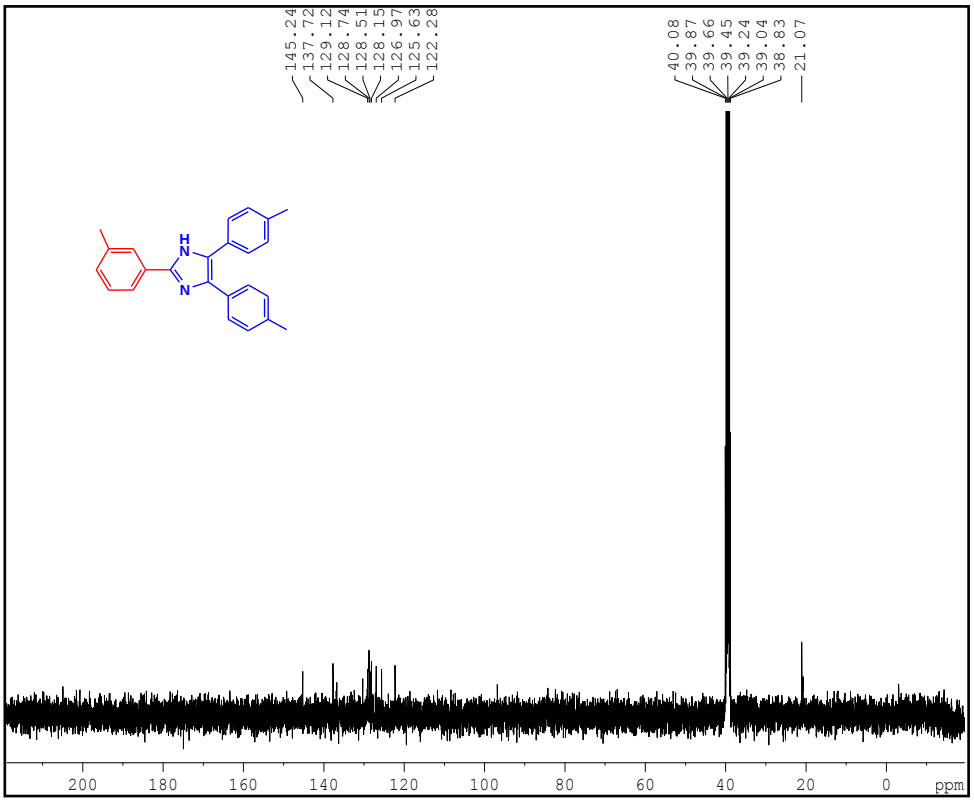
[1]H NMR (400 MHz, DMSO-*d6*) spectrum of 5o(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



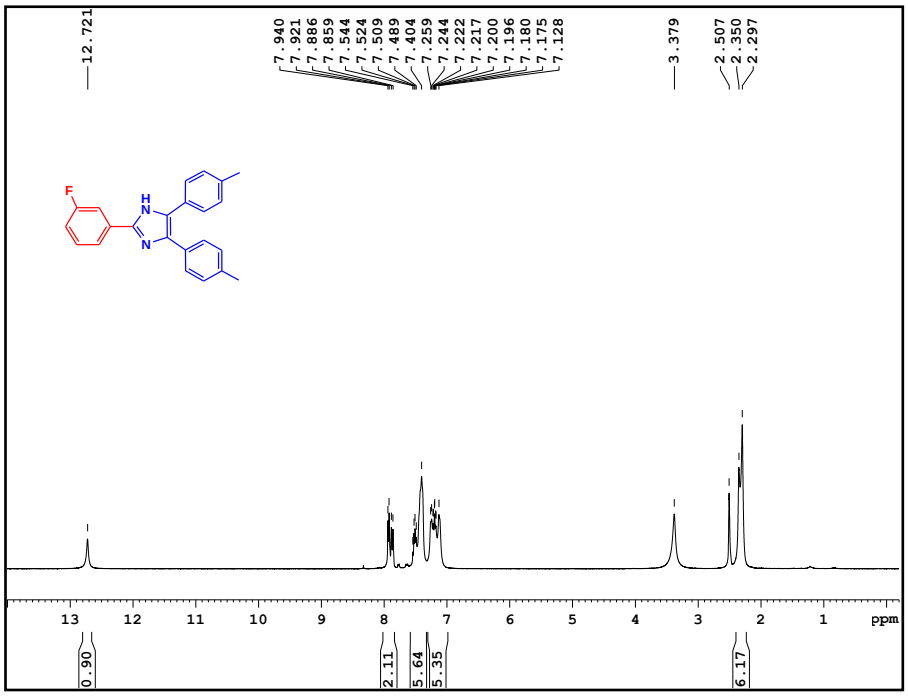
[13]C NMR (100 MHz, DMSO-*d6*) spectrum of 5o



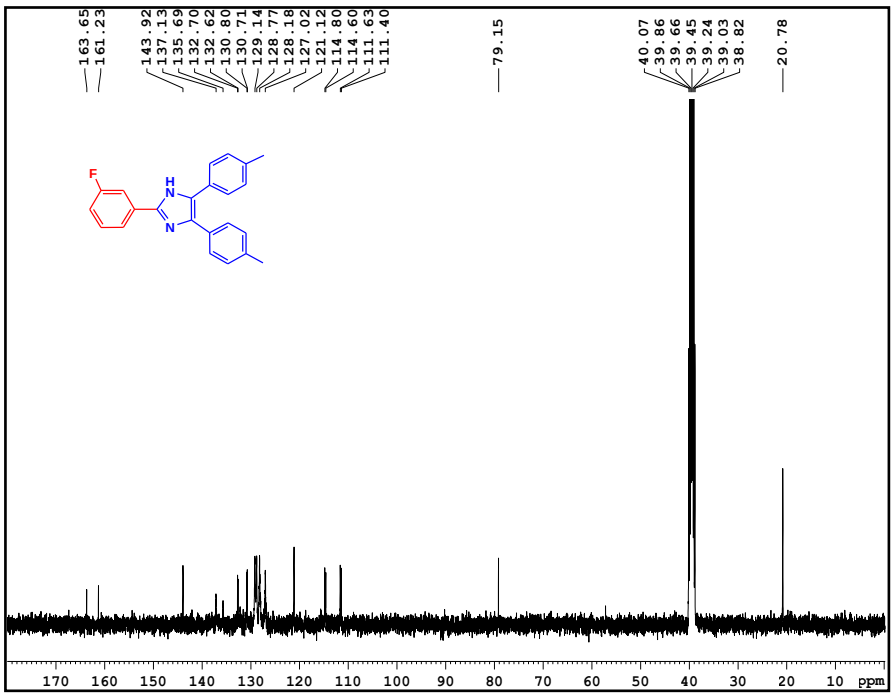
^{1}H NMR (400 MHz, DMSO-*d6*) spectrum of 5p(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



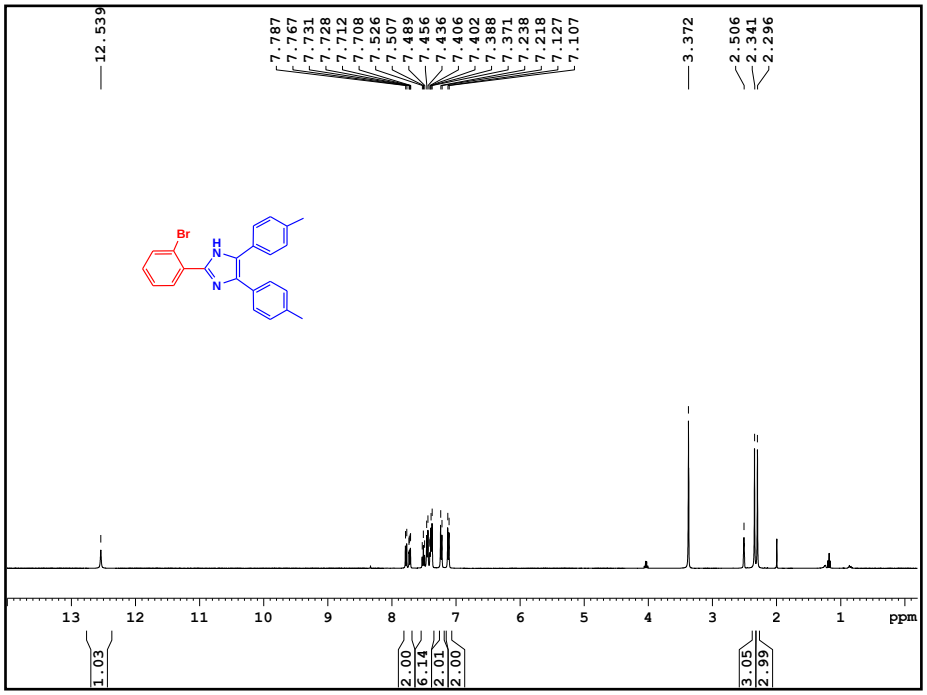
^{13}C NMR (100 MHz, DMSO-*d6*) spectrum of 5p



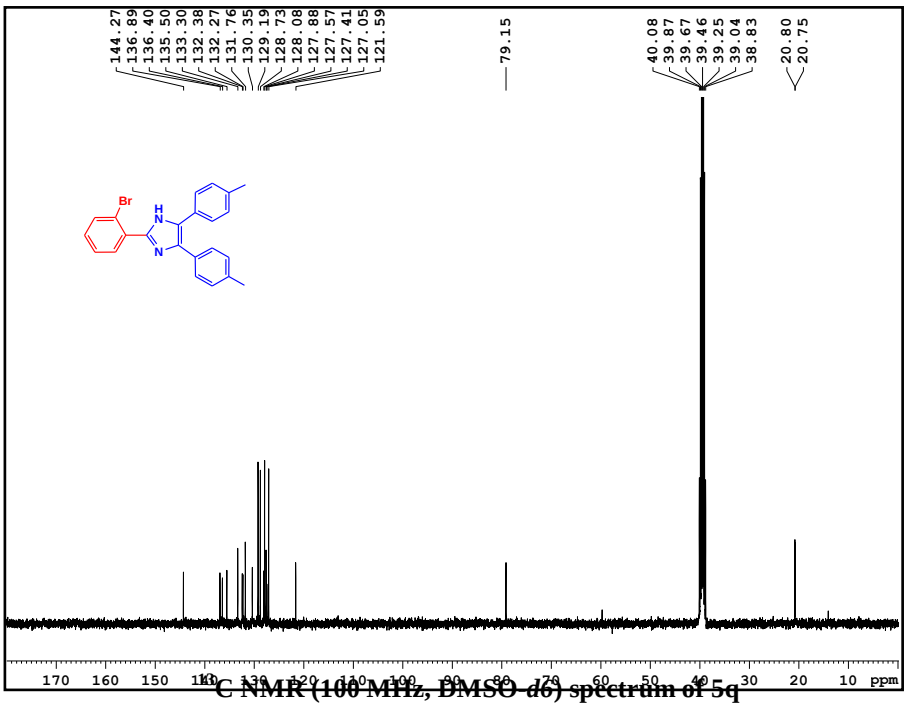
[1]H NMR (400 MHz, DMSO-*d6*) spectrum of 5q(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



[13]C NMR (100 MHz, DMSO-*d6*) spectrum of 5q



^{1}H NMR (400 MHz, DMSO-*d6*) spectrum of 5r(peaks at 3.3 and 2.5 ppm are solvent and water peaks)



^{13}C NMR (100 MHz, DMSO-*d6*) spectrum of 5q

^{13}C NMR (100 MHz, DMSO-*d6*) spectrum of 5r

4. X-ray crystal data and structural determination of complex 2

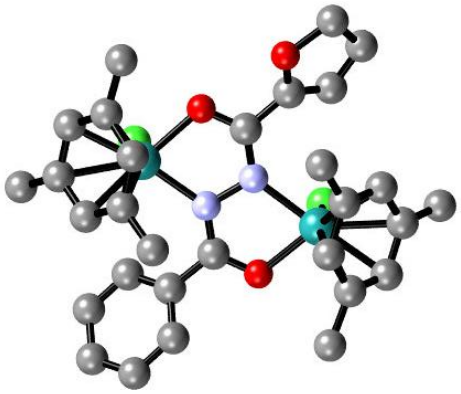


Figure S1. X-ray crystal structure of complex **2**

Table S1:

CCDC	1849212
Chemical formula	$C_{30}H_{32}Cl_2N_2O_3Ru_2 \cdot CH_2Cl_2$
M_r	826.54
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	16.6576 (8), 13.2575 (6), 15.4394 (7)
β (°)	109.200 (2)
V (Å^3)	3220.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.31
Crystal size (mm)	0.19 × 0.11 × 0.07
Diffractometer	Bruker *APEX*-II CCD diffractometer
Absorption correction	Multi-scan*SADABS*(Sheldrick, 1996)
T_{min}, T_{max}	0.677, 1.000
No. of measured, independent and observed [I> 2σ(I)] reflections	29702, 7766, 6446
R_{int}	0.024
(sin θ/λ)$_{max}$ (Å^{-1})	0.662

Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.121, 1.05
No. of reflections	7766
No. of parameters	373
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.83, −1.10