Electronic Supplementary Information (ESI)

Synthesis, crystal structure and water oxidation activity of $[Ru(terpy)(bipy)Cl]^+$ complexes: Influence of ancillary ligands on O_2 generation

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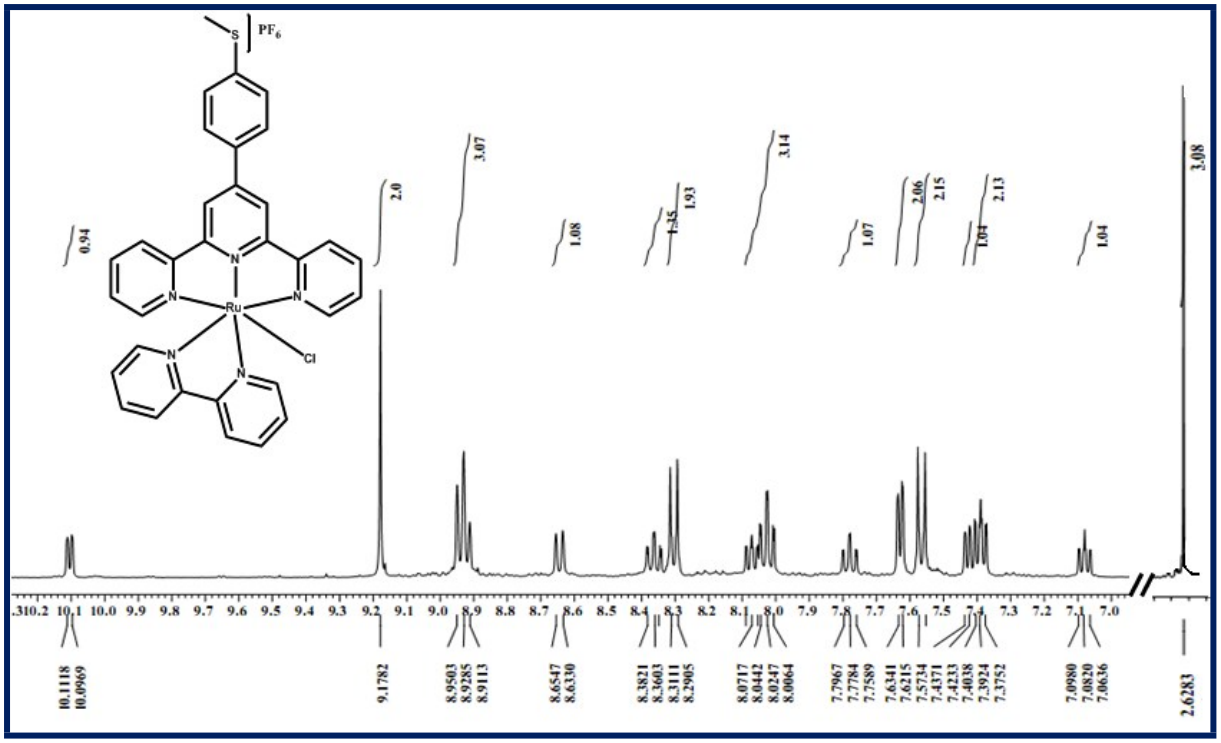


Fig. S1: ^{1}H NMR spectrum of complex **1** in DMSO-d_6

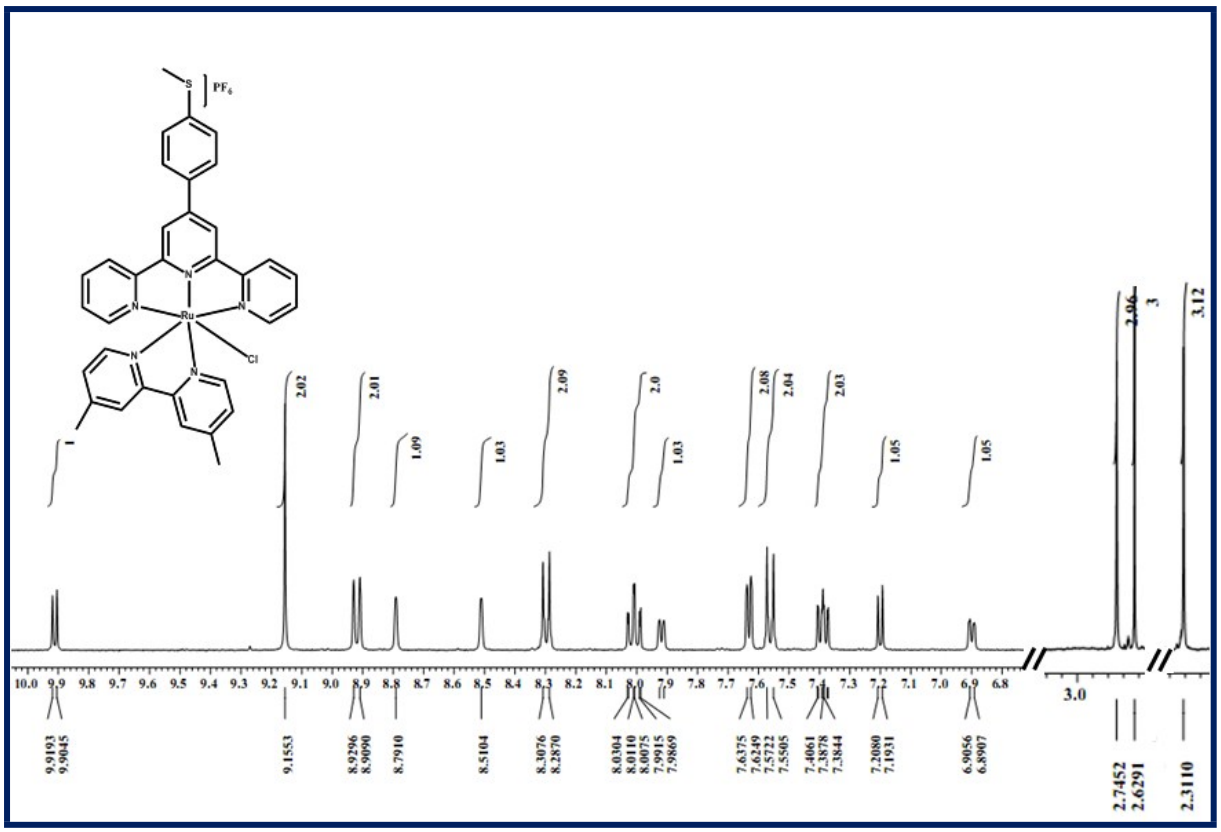


Fig. S2: ^{1}H NMR spectrum of complex 2 in DMSO-d_6

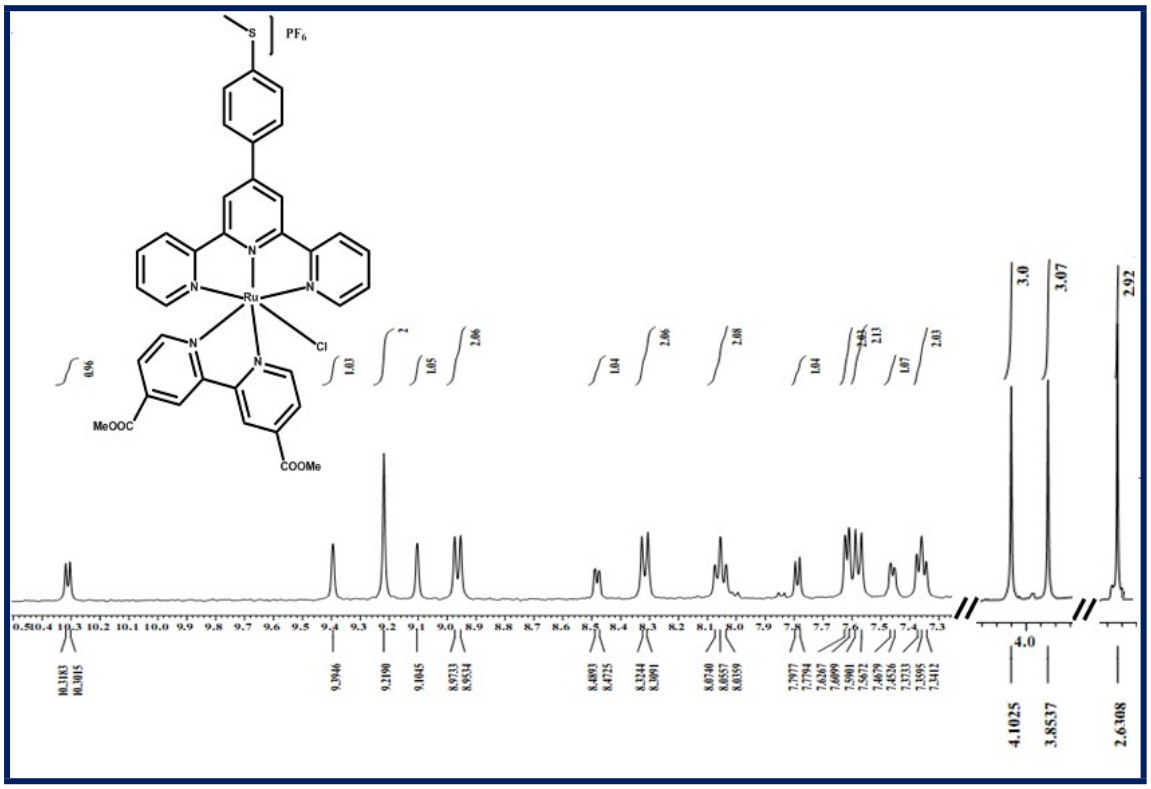


Fig. S3: ^{1}H NMR spectrum of complex 3 in DMSO-d_6

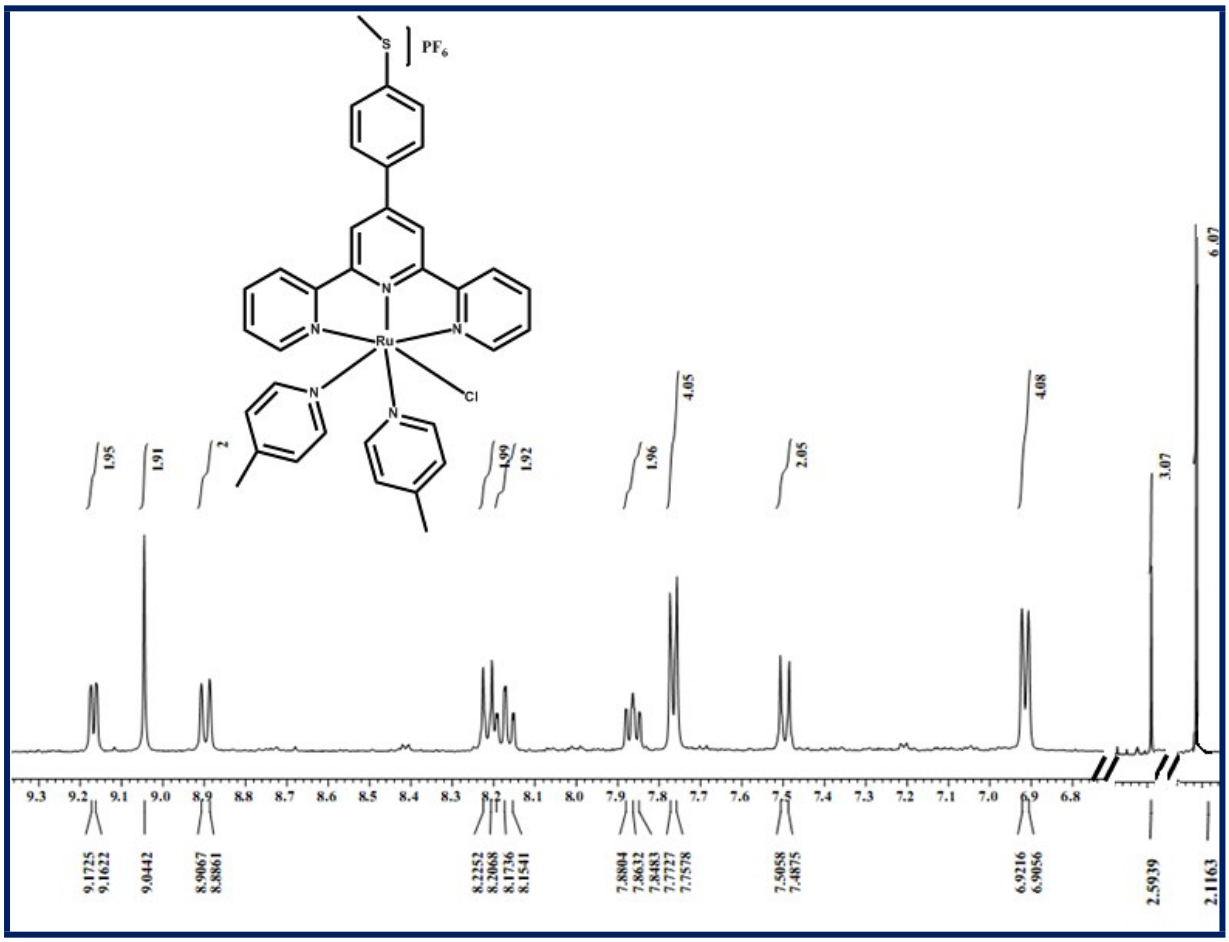


Fig. S4: ^{1}H NMR spectrum of complex **4** in DMSO-d_6

Table S1: Selected bond distances (Å) and angles (°) for complexes **1** &**2**

Complex **1**			
Ru1-N1	2.078(6)	Ru1-N5	2.066(6)
Ru1-N2	2.042(6)	Ru1-N6	1.942(6)
Ru1-N3	2.065(6)	Ru1-Cl1	2.410(19)
Cl1-Ru1-N1	95.33(17)	N1-Ru1-N6	172.7(2)
Cl1-Ru1-N2	170.01(16)	N2-Ru1-N3	87.4(2)
Cl1-Ru1-N3	88.74(17)	N2-Ru1-N5	96.7(2)
Cl1-Ru1-N5	89.37(17)	N2-Ru1-N6	95.0(2)
Cl1-Ru1-N6	91.15(16)	N3-Ru1-N5	159.0(2)
N1-Ru1-N2	78.9(2)	N3-Ru1-N6	79.2(2)
N1-Ru1-N3	104.2(2)	N5-Ru1-N6	79.9(2)
N1-Ru1-N5	96.9(2)		
Complex **2**			
Ru1-N1	2.070(3)	Ru1-N4	2.040(2)
Ru1-N2	1.951(3)	Ru1-N5	2.060(3)
Ru1-N3	2.084(3)	Ru1-Cl1	2.413(13)
Cl1-Ru1-N1	89.54(6)	N1-Ru1-N5	159.32(10)
Cl1-Ru1-N2	90.34(7)	N2-Ru1-N3	173.40(10)
Cl1-Ru1-N3	94.85(6)	N2-Ru1-N4	96.42(9)
Cl1-Ru1-N4	173.24(7)	N2-Ru1-N5	79.80(10)
Cl1-Ru1-N5	89.95(6)	N3-Ru1-N4	78.40(9)
N1-Ru1-N2	79.53(10)	N3-Ru1-N5	96.10(10)
N1-Ru1-N3	104.54(10)	N4-Ru1-N5	91.17(9)
N1-Ru1-N4	91.76(9)		

Table S2: First order rate data

Complex	K x 10^{-3}	R*	$t_{1/2}$
1	**9.0**	**0.9957**	**77**
2	**4.5**	**0.9966**	**154**
3	**1.8**	**0.9987**	**384**
4	**5.3**	**0.9973**	**130**

* R indicates the goodness of fit to a linear trace.

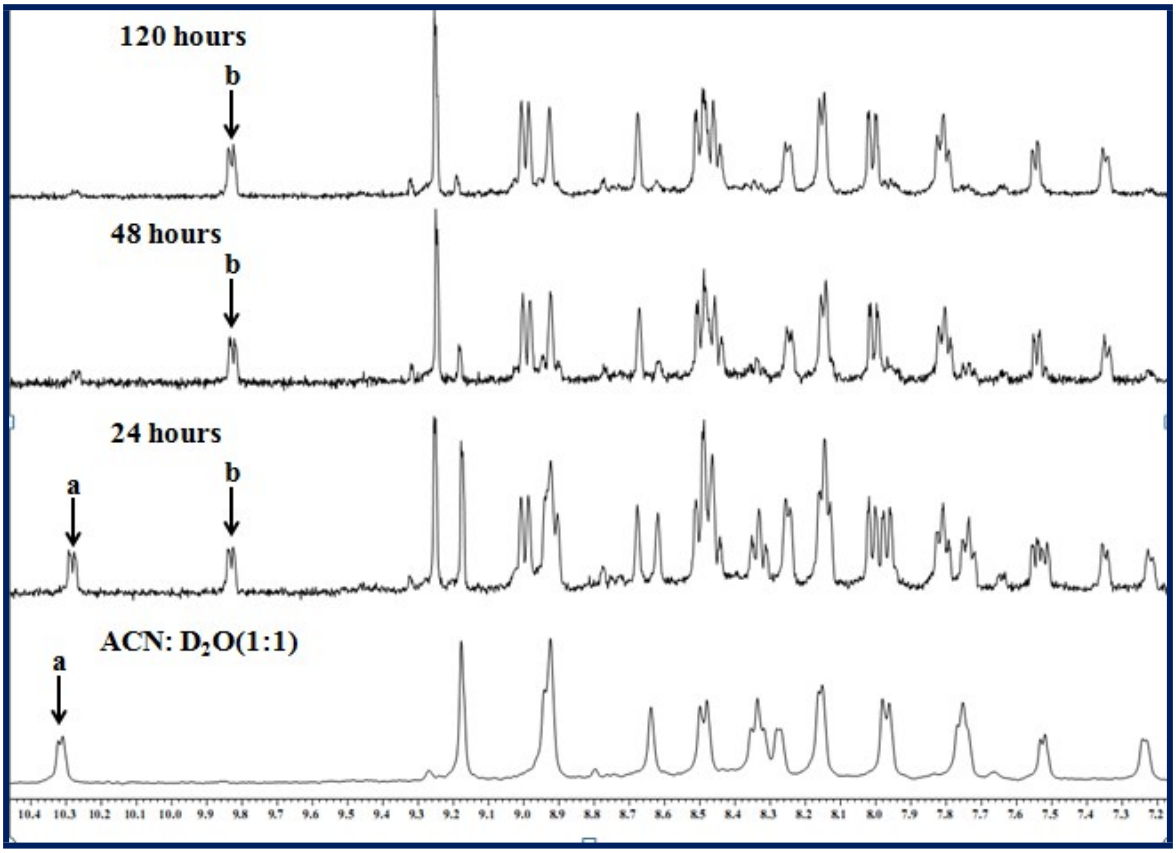


Fig. S5: ^{1}H NMR stack plot of complex **2** in 1:1 ACN-d_3/D_2O mixture with labeling of the peak due to H11 proton (a) adjacent to (chlorido), (b) adjacent to (aqua) ligand.

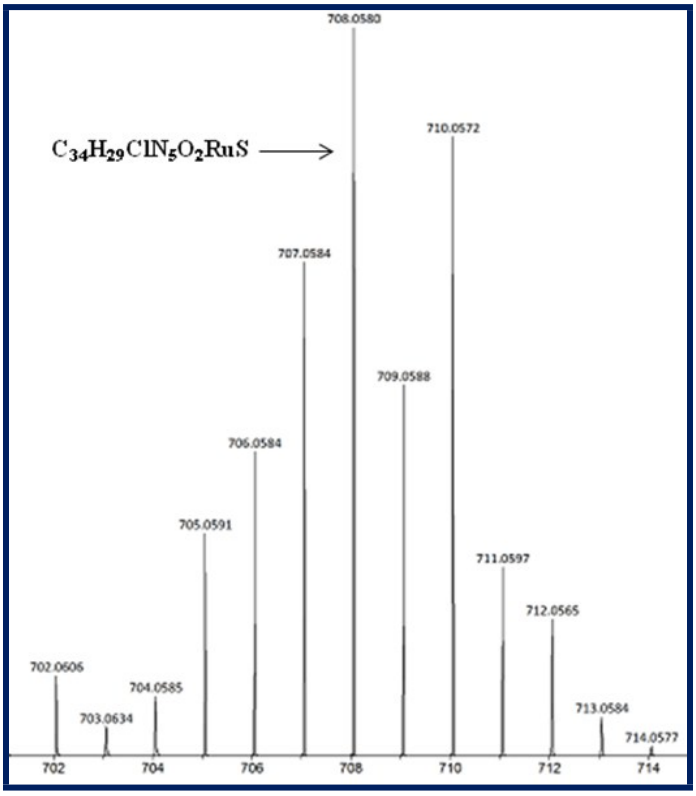
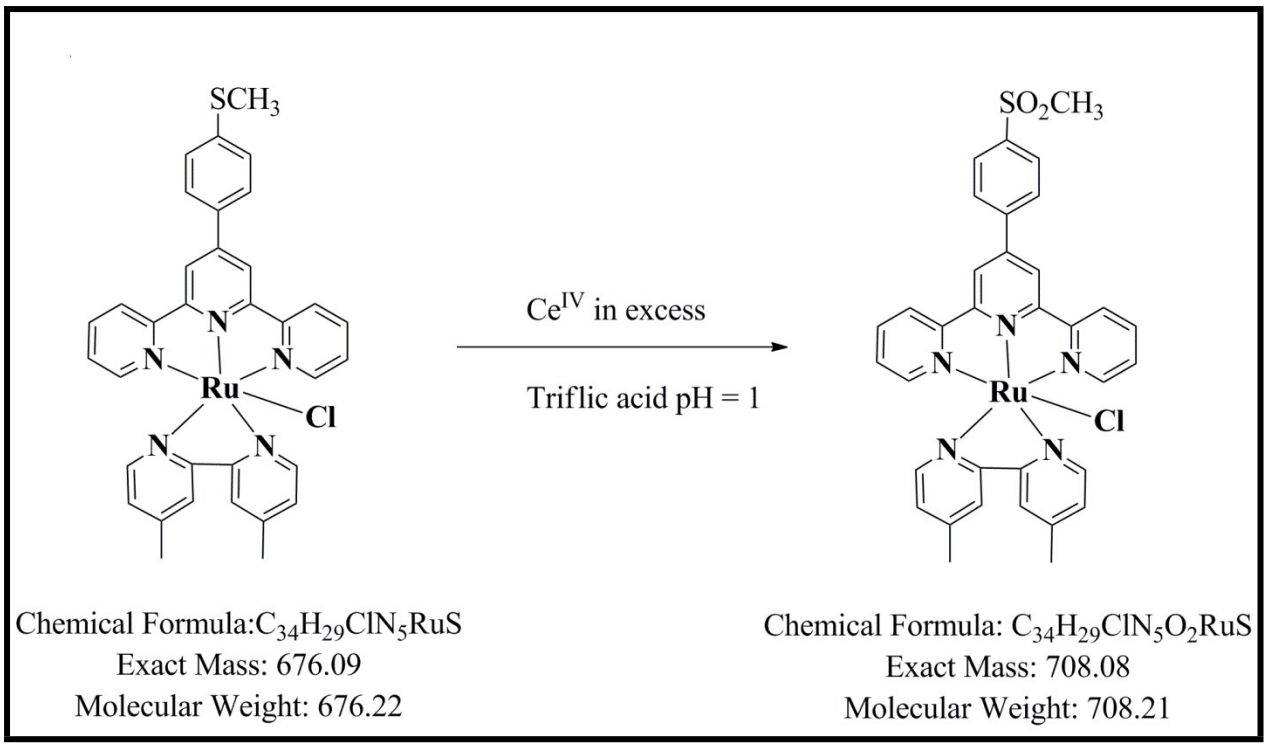


Fig. S6: ESI-MS spectrum of isolated complex **2** after oxidation with CAN showing the molecular ion peak at m/z 708.077.



Scheme S1: Regeneration of the catalyst **2** involving the oxidation of the MeMPTP ligand

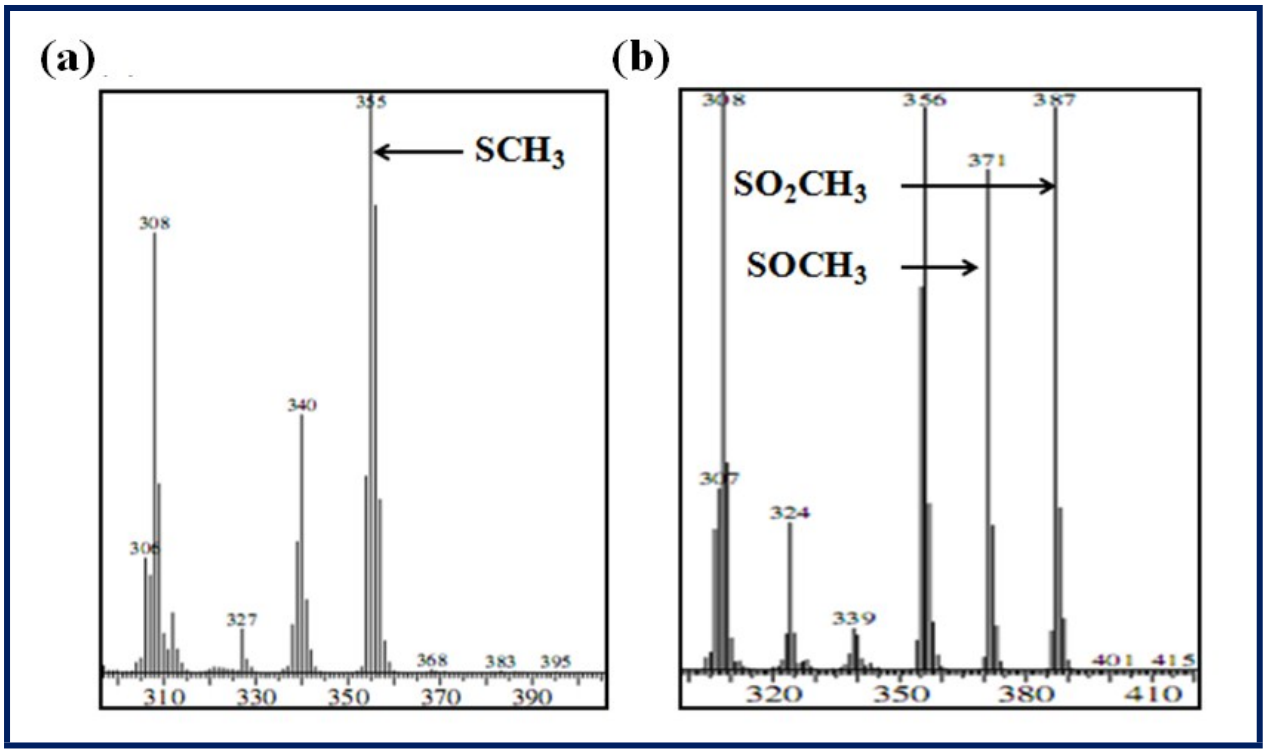


Fig. S7: ESI-MS spectra of MeMPTP ligand before (a) and after (b) treating with CAN.