

Supplementary Material

Syntheses and Characterization of Oxo-centered Triruthenium Compounds with Orthometallated Bipyridine

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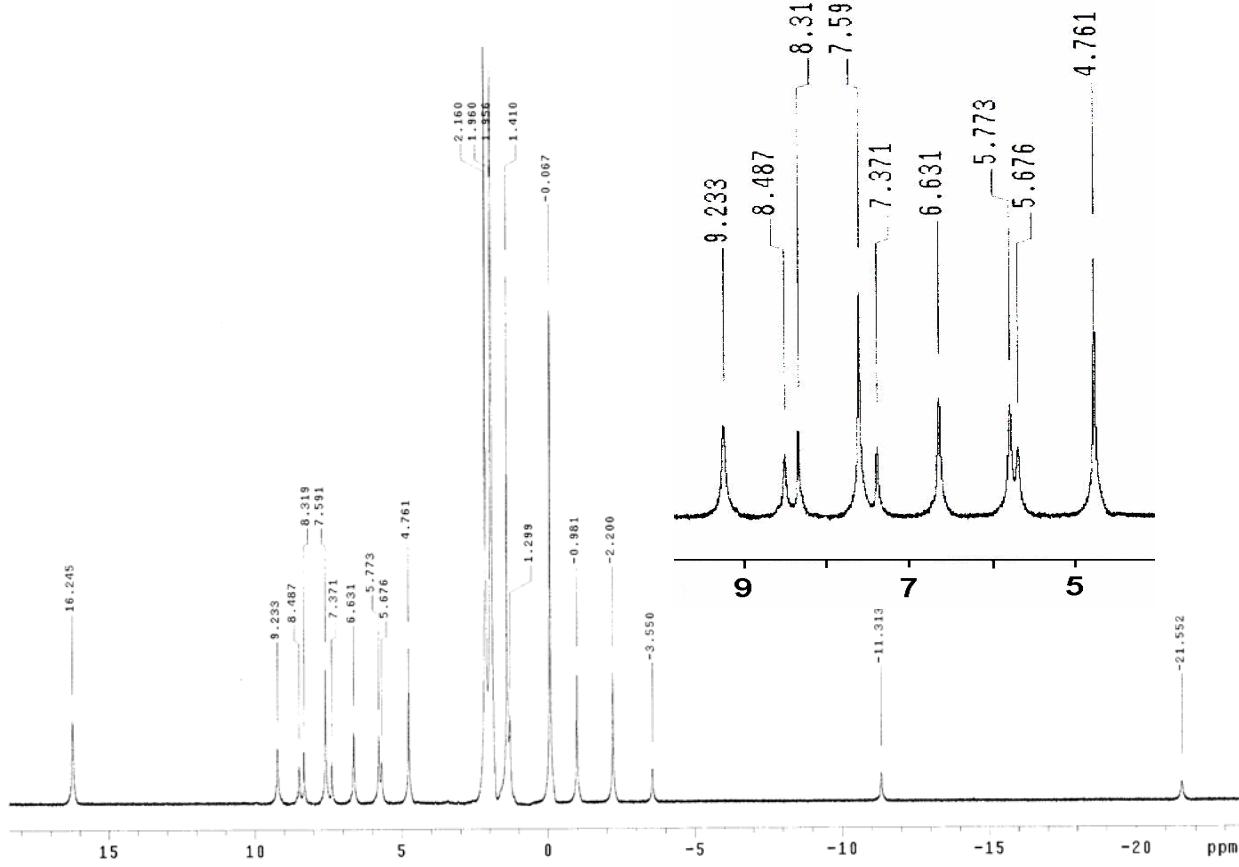


Figure S1. ^1H NMR (499.8 MHz) spectrum of **2** in CD_3CN .

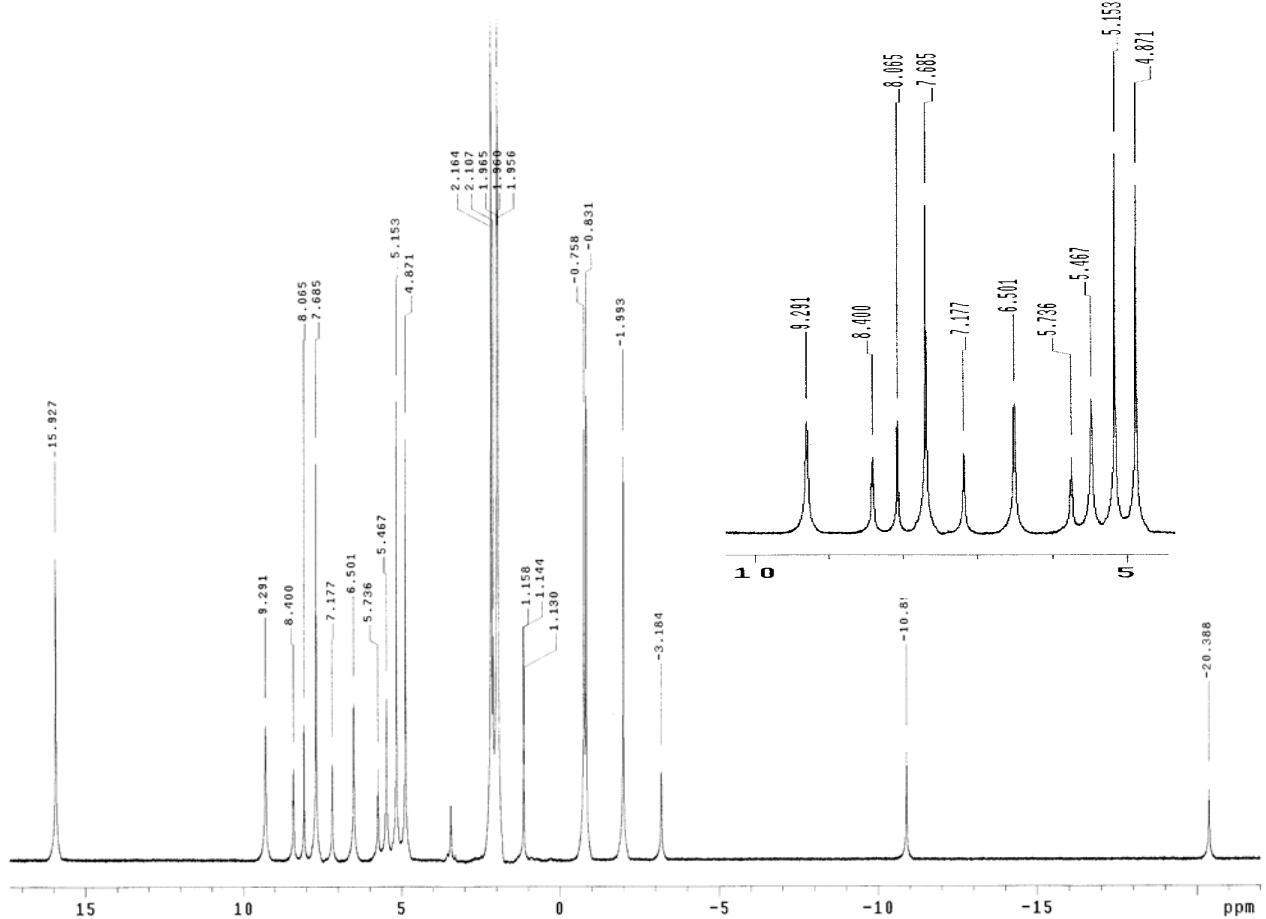


Figure S2. ^1H NMR (499.8 MHz) spectrum of **3** in CD_3CN .

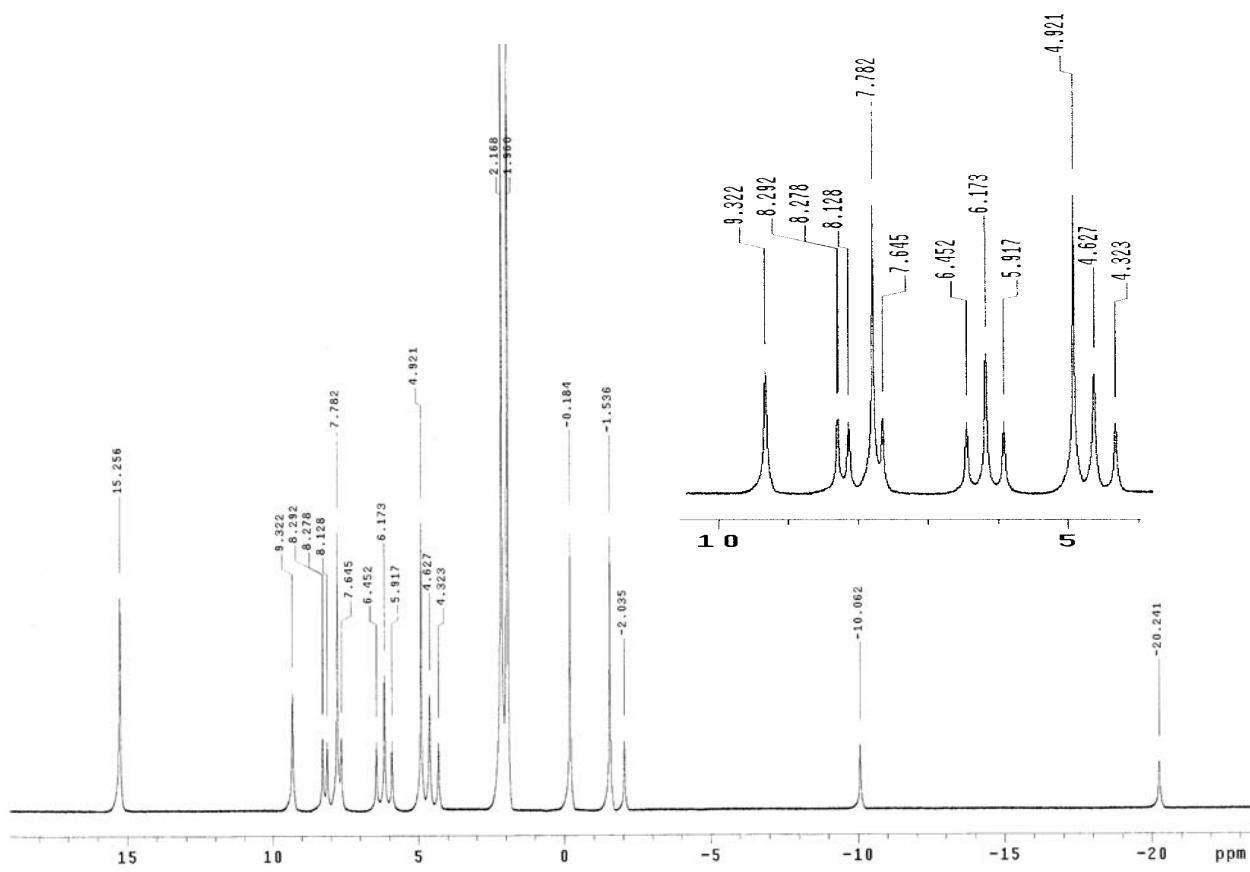


Figure S3. ^1H NMR (499.8 MHz) spectrum of **4** in CD_3CN .

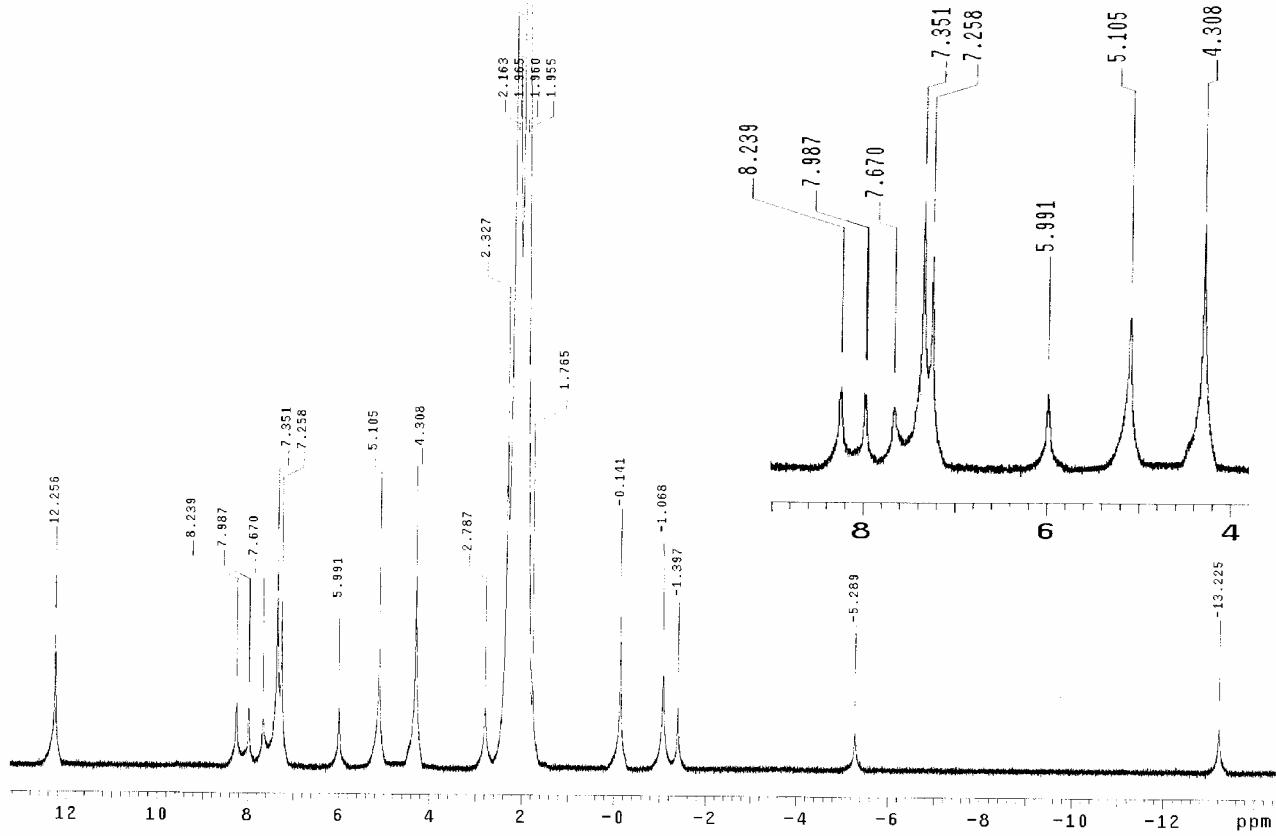


Figure S4. ^1H NMR (499.8 MHz) spectrum of **5** in CD_3CN .

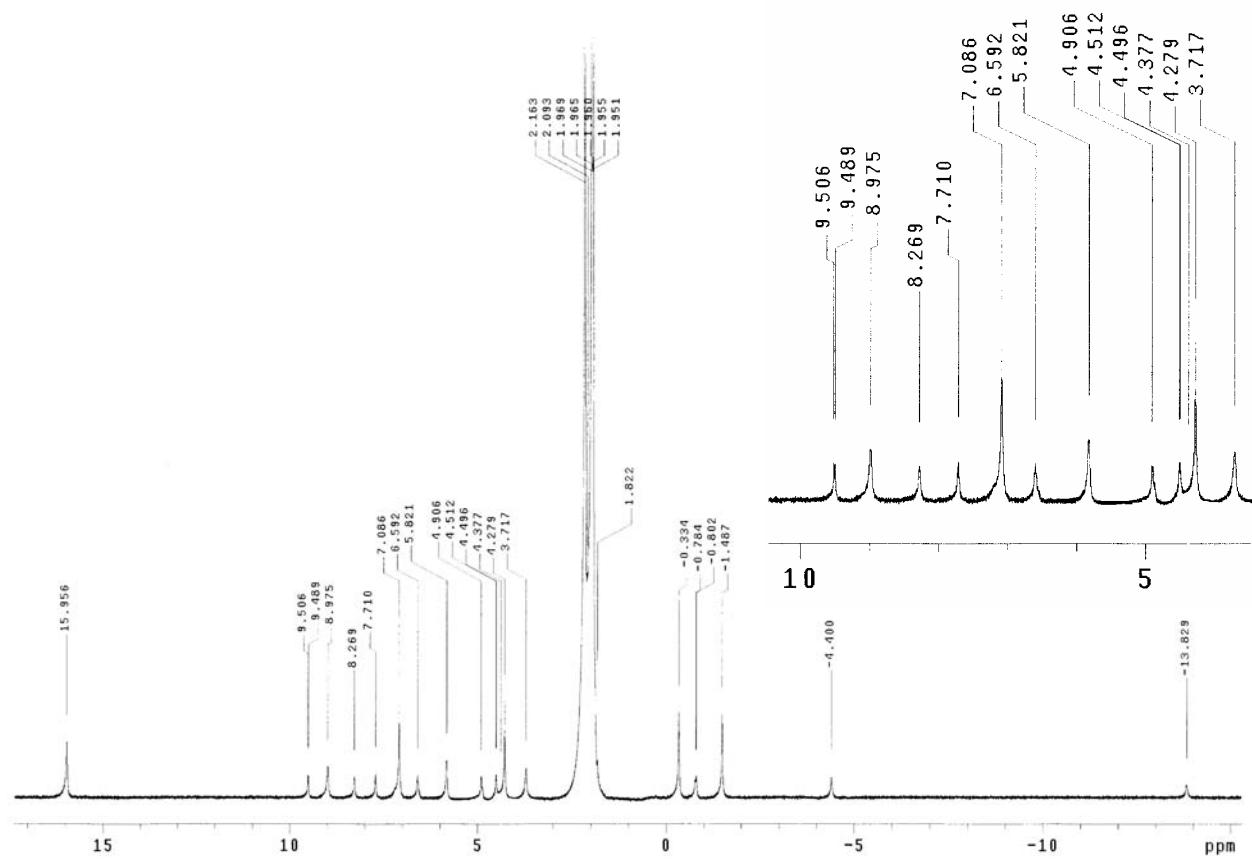


Figure S5. ¹H NMR (499.8 MHz) spectrum of **6** in CD₃CN.

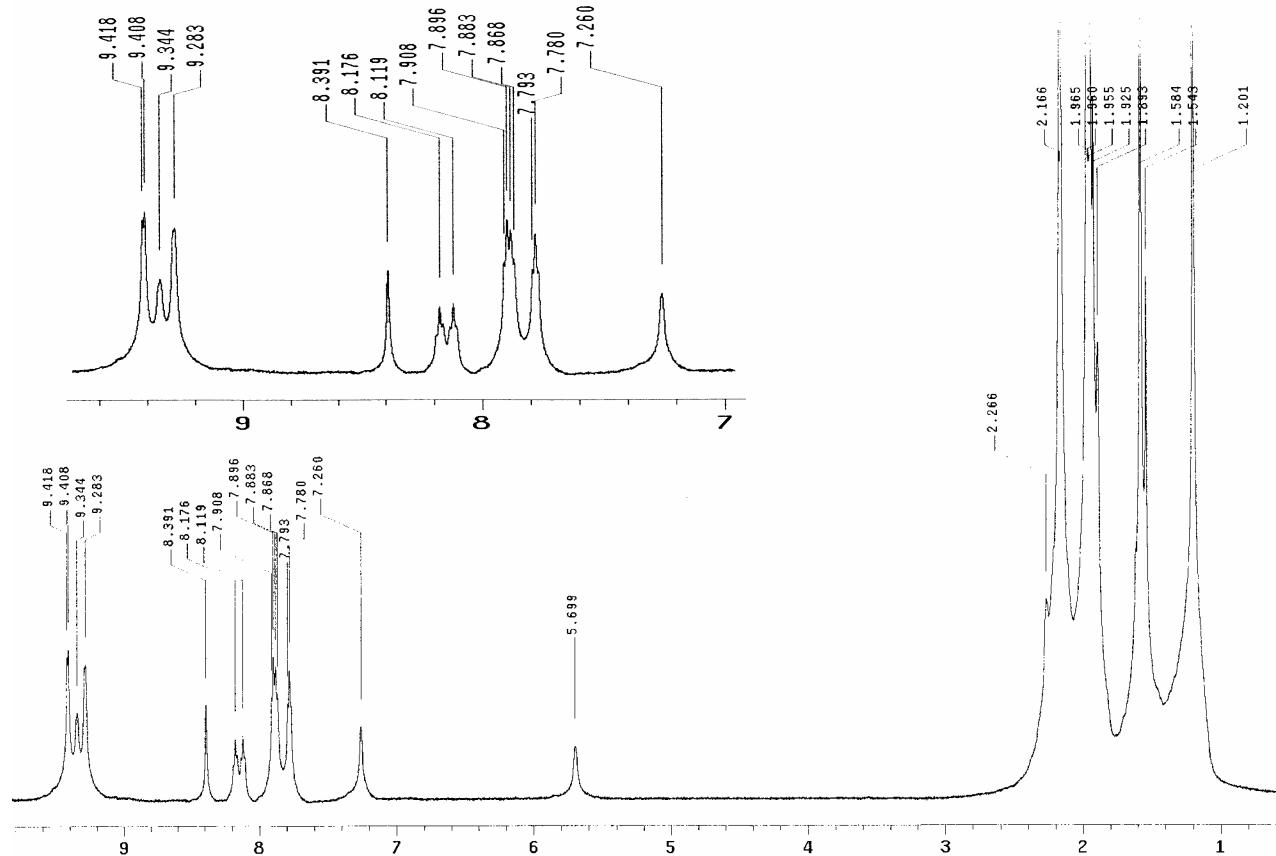


Figure S6. ¹H NMR (499.8 MHz) spectrum of **2a** in CD₃CN

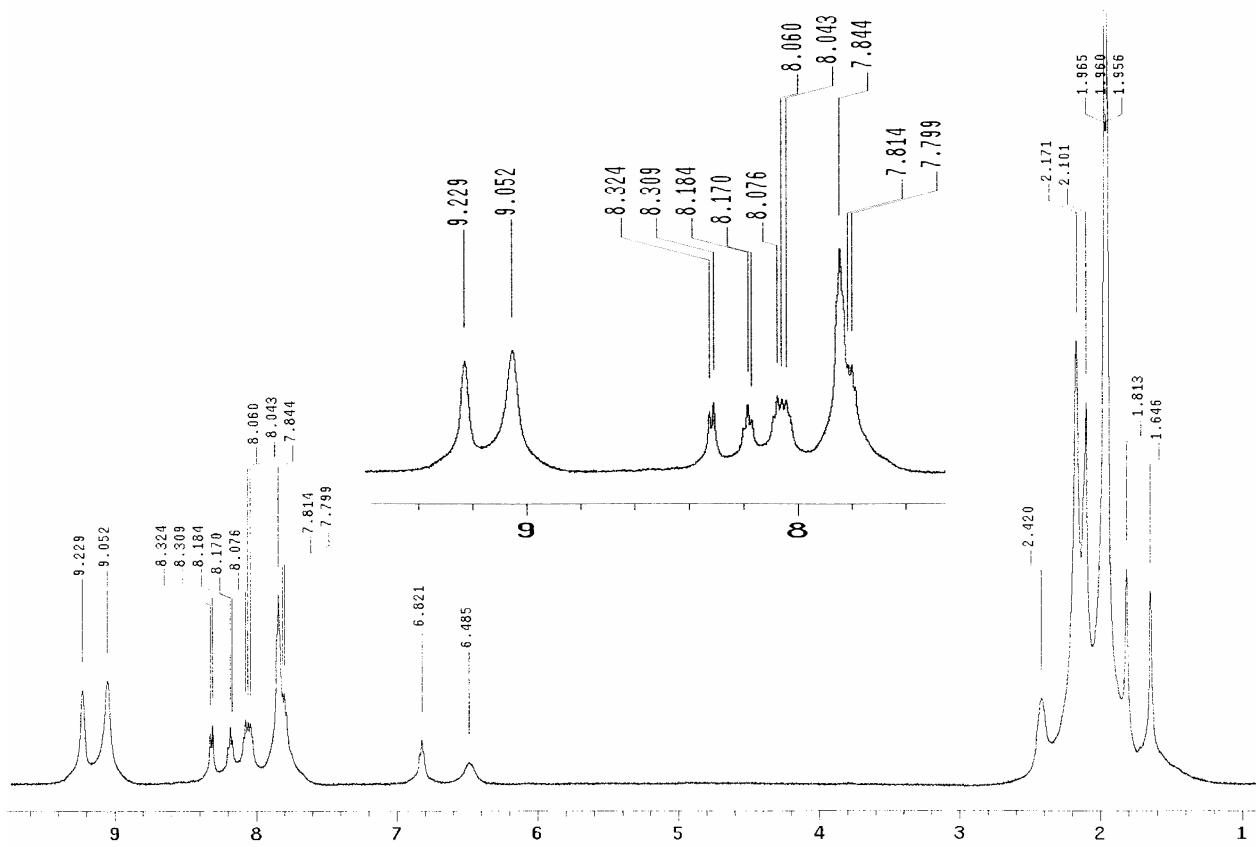
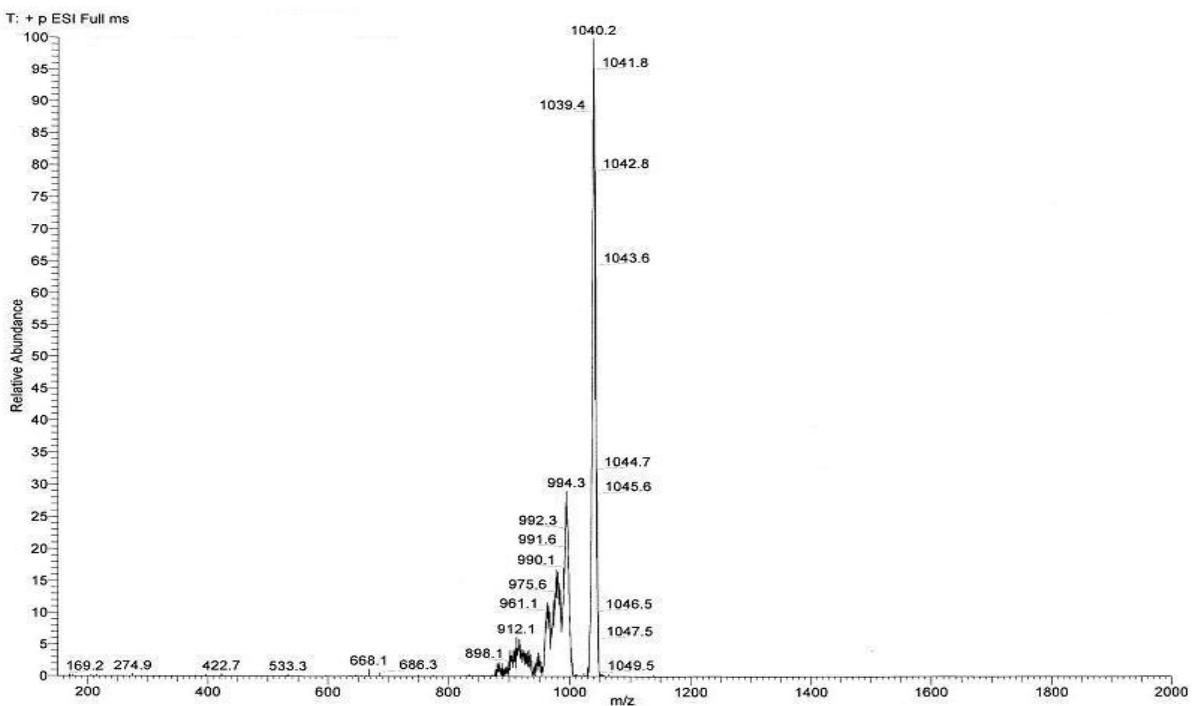


Figure S7. ¹H NMR (499.8 MHz) spectrum of **4a** in CD₃CN



Positive ion fragments m/z (%):

1041 (100): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{py})_2(\text{Bu}_2\text{bpy}^-)]^+$

994 (30): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{py})(\text{Bu}_2\text{bpy}^-)(\text{MeOH})]^+$

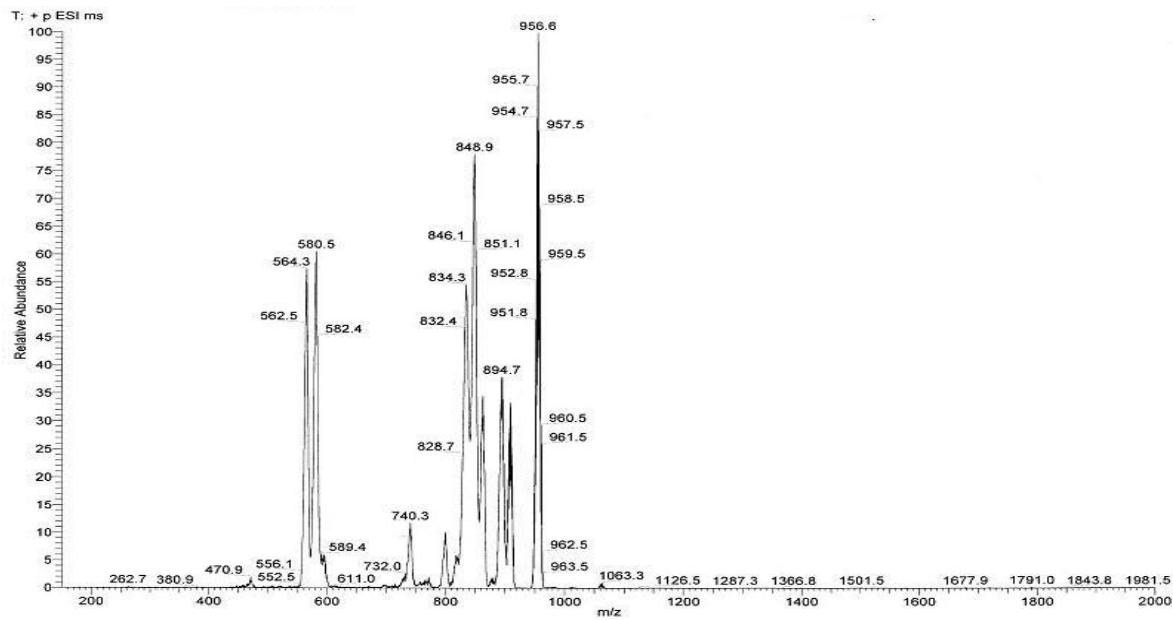


Figure S9. ES-MS of compound 3.

Positive ion fragments m/z (%):

957 (100): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{py})_2(\text{Me}_2\text{bpy}^-)]^+$

849 (80): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{Me}_2\text{bpy}^-)(\text{MeOH})(\text{H}_2\text{O})]^+$

835 (55): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{Me}_2\text{bpy}^-)(\text{H}_2\text{O})_2]^+$

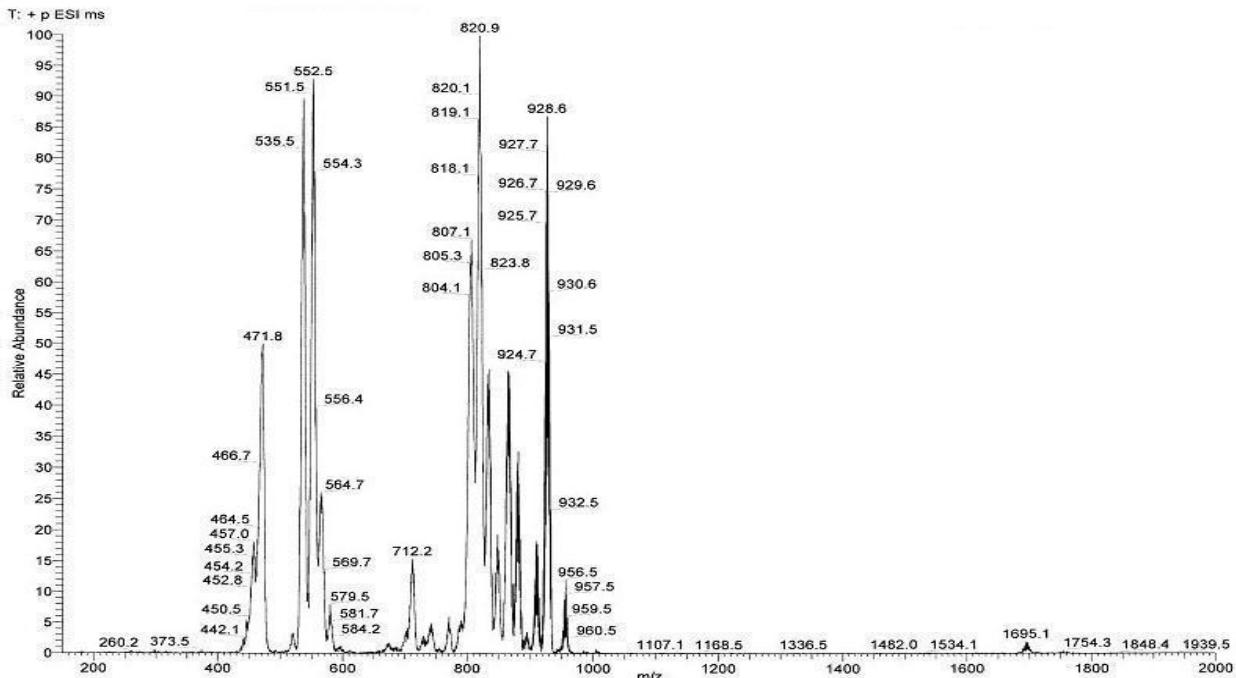


Figure S10. ES-MS of compound 4.

Positive ion fragments m/z (%):

- 929 (88): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{py})_2(\text{bpy}^-)]^+$
 835 (45): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{bpy}^-)(\text{MeOH})_2]^+$
 821 (100): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{bpy}^-)(\text{MeOH})(\text{H}_2\text{O})]^+$
 807 (67): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{bpy}^-)(\text{H}_2\text{O})_2]^+$

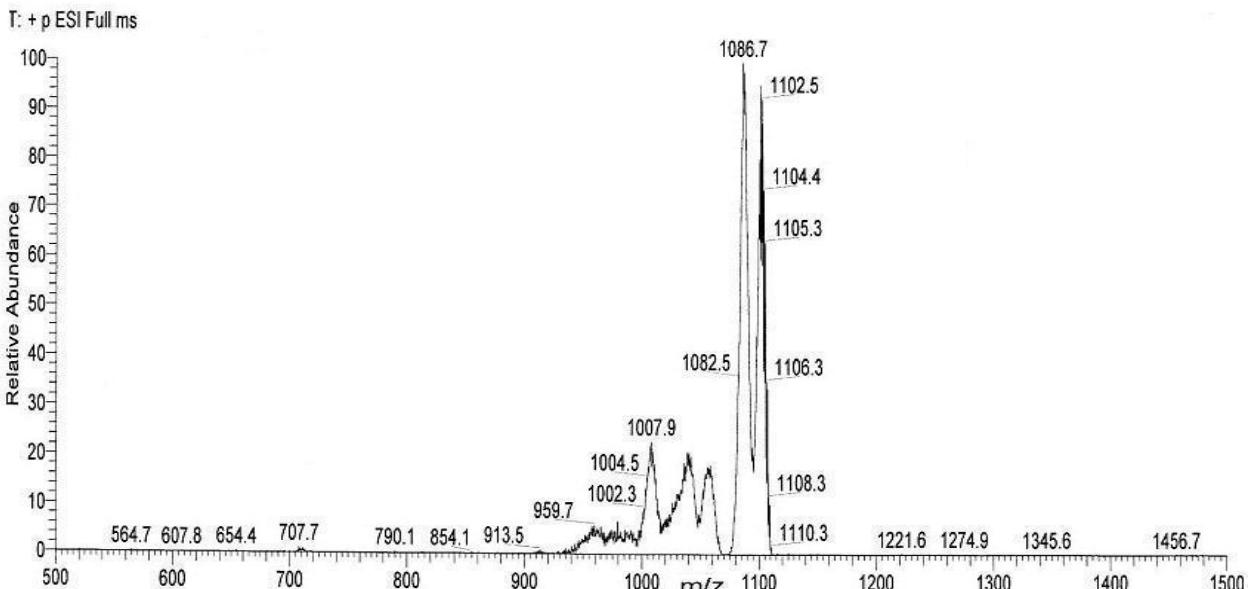


Figure S11. ES-MS of compound 5.

Positive ion fragments m/z (%):

- 1105 (92): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{py})_2(\text{Br}_2\text{bpy}^-)(\text{H}_2\text{O})]^+$
 1087 (100): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{py})_2(\text{Br}_2\text{bpy}^-)]^+$

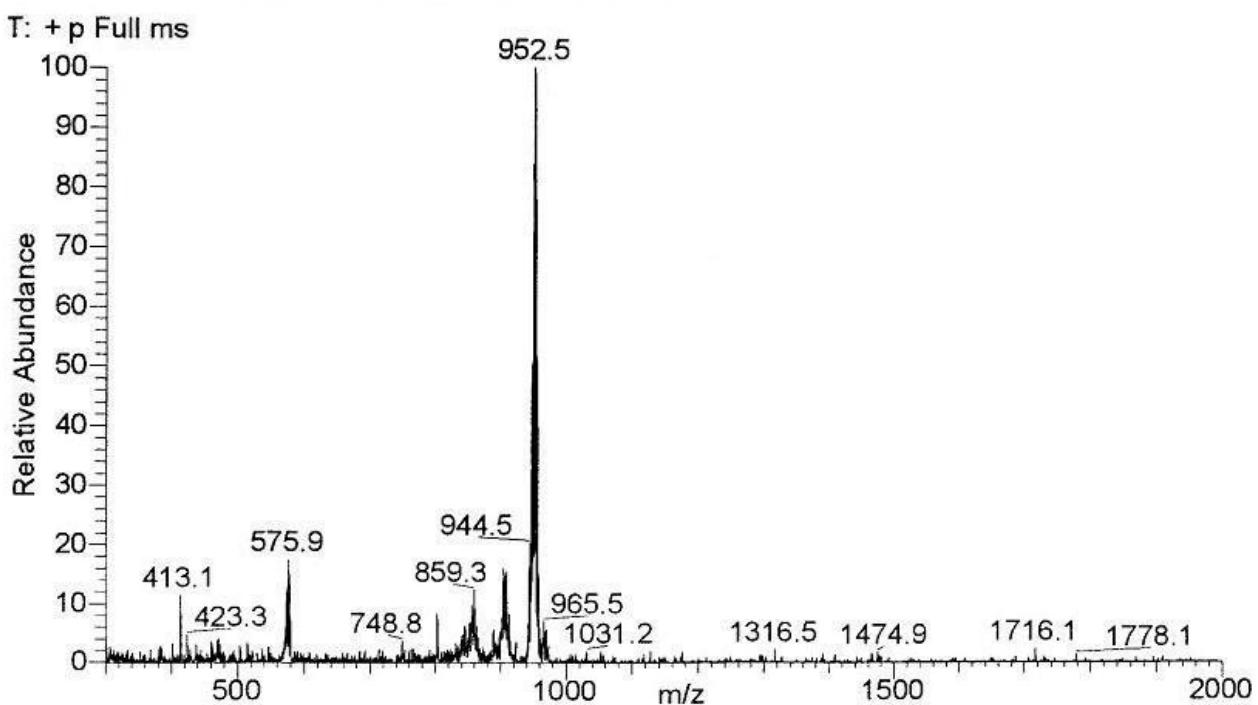


Figure S12. ES-MS of compound 6.

Positive ion fragments m/z (%):

953 (100): $[\text{Ru}_3\text{O}(\text{OAc})_5(\text{py})_2(\text{phen}^-)]^+$