Supplementary Information

for

Acetal-functionalised RAPTA complexes for conjugation and labeling

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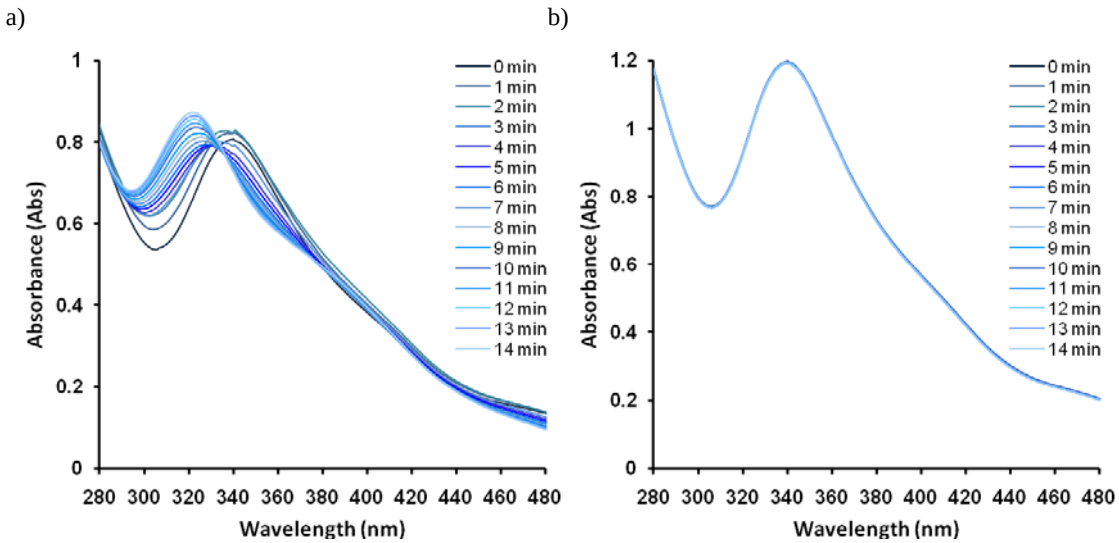


Figure S1. Time-course UV absorption spectra of **4** in H_2O (left); and 150 mM NaCl (right).

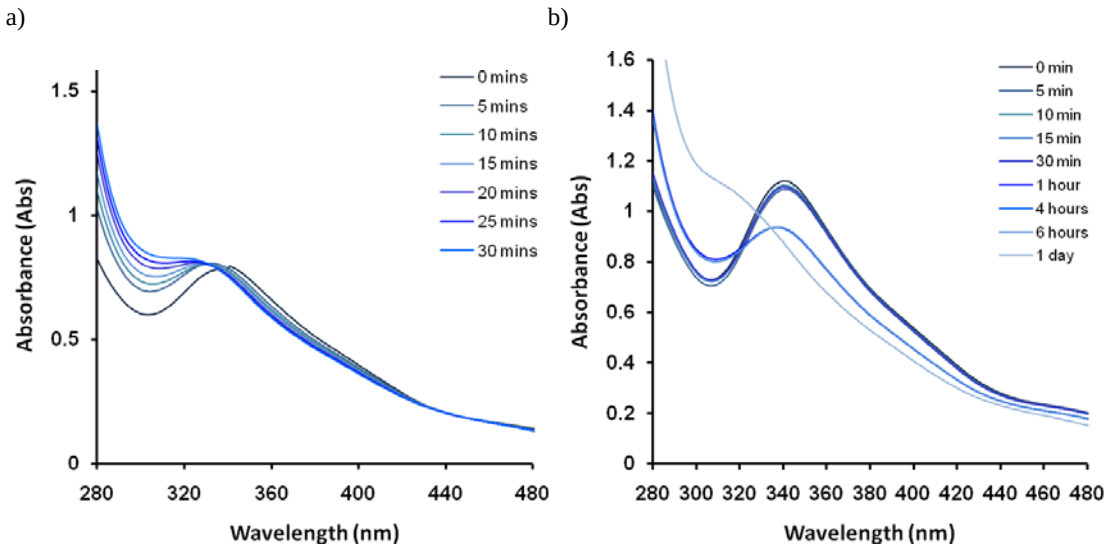


Figure S2. Time course UV-vis absorption spectra of **4** in 1 mM GSH (left); and 150 mM NaCl /1 mM GSH (right).

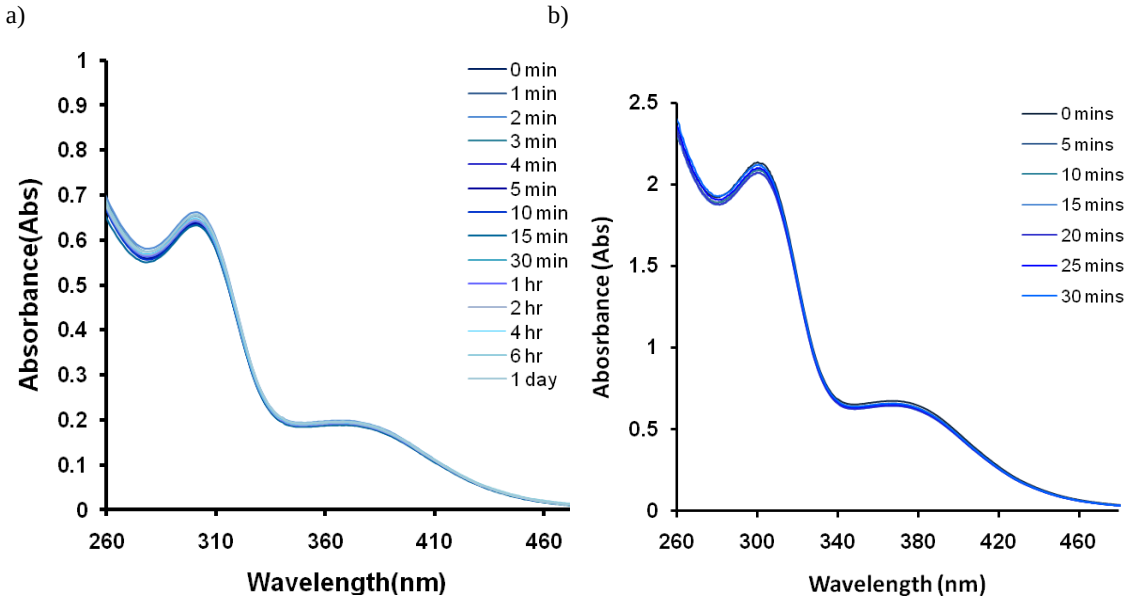


Figure S3. Time-course UV absorption spectra of **5** in H_2O (left); and 1 mM GSH (right).

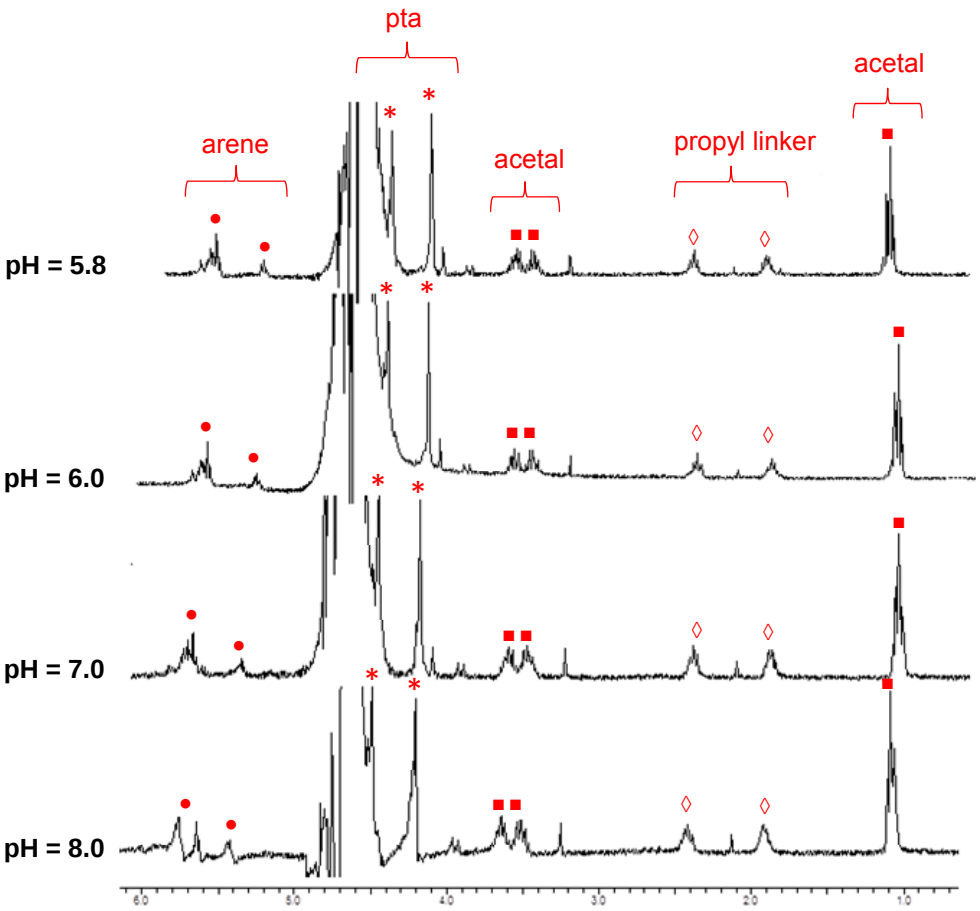
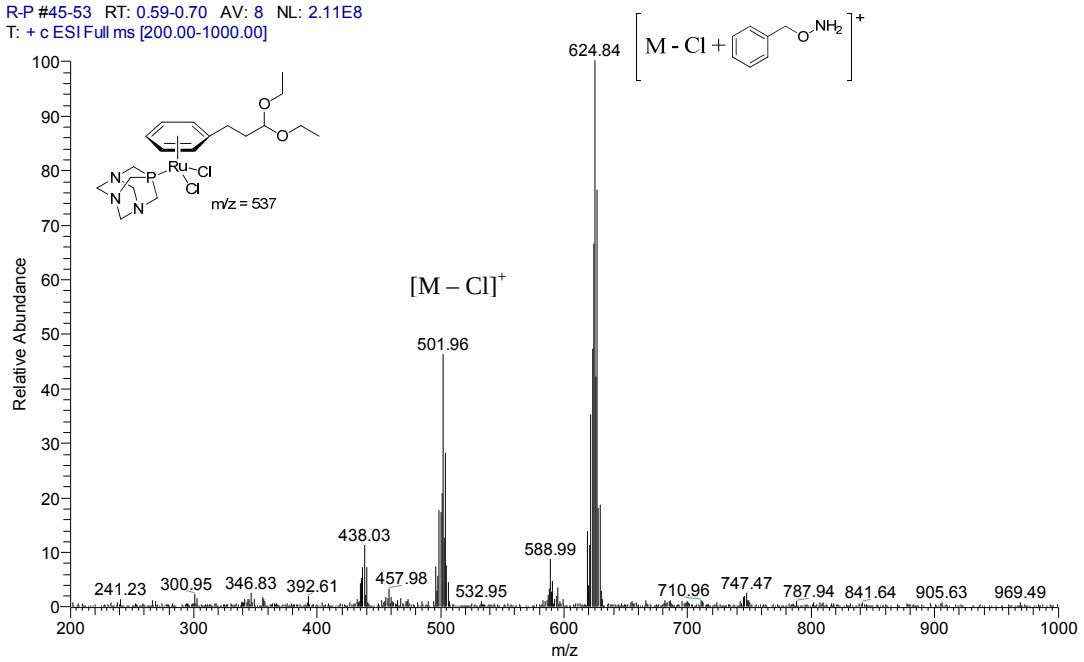


Figure S4. ^{1}H NMR spectrum of **5** in D_2O under different pH conditions.

a)



b)

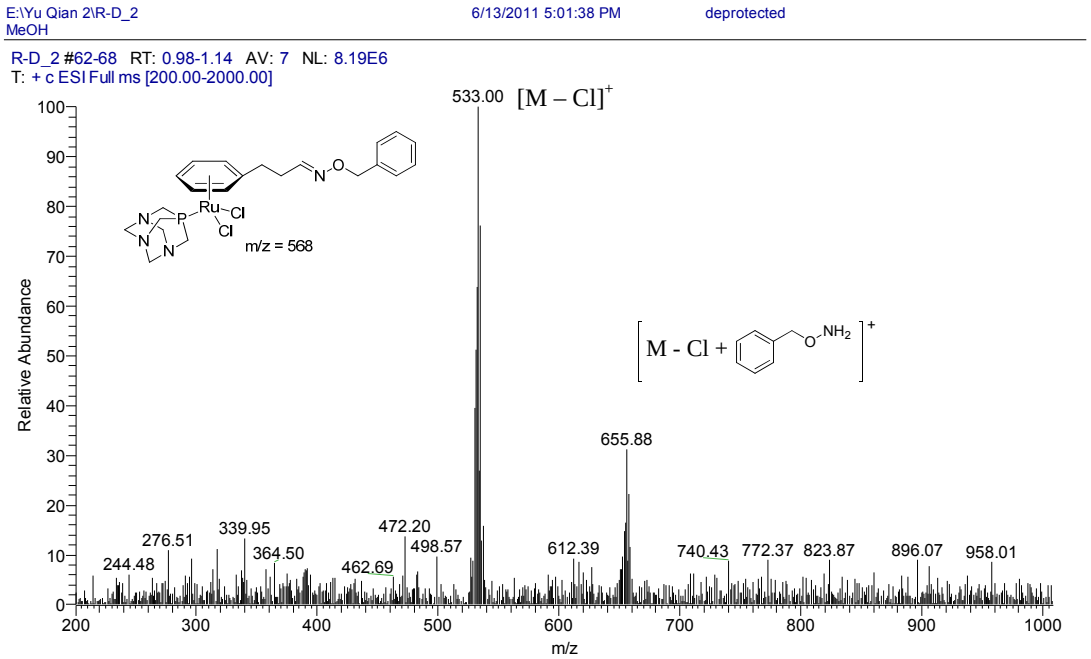
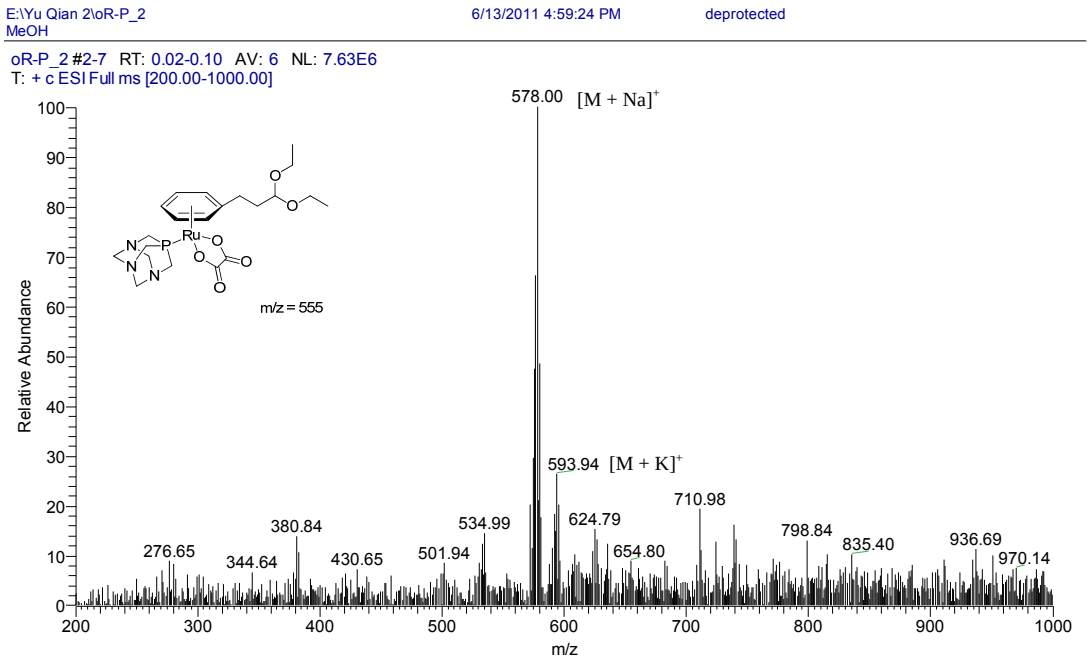


Figure S5. ESI-MS spectra of conjugation reaction of (a) protected **4** with *o*-benzylhydroxylamine; (b) deprotected **4** (treated with 10 mM HCl) with *o*-benzylhydroxylamine

a)



b)

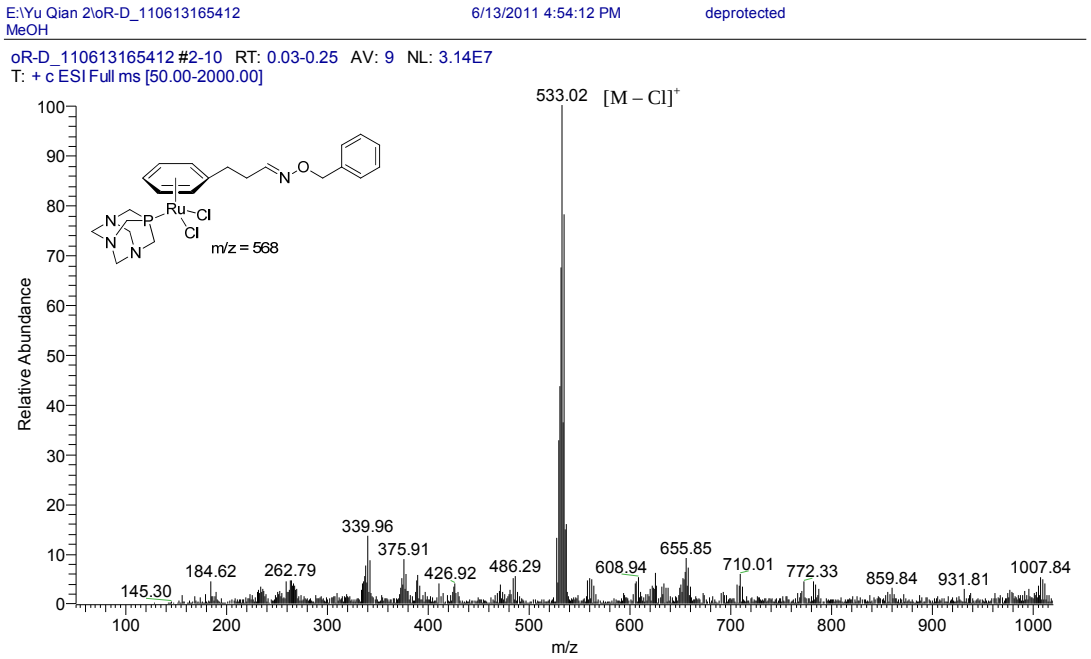
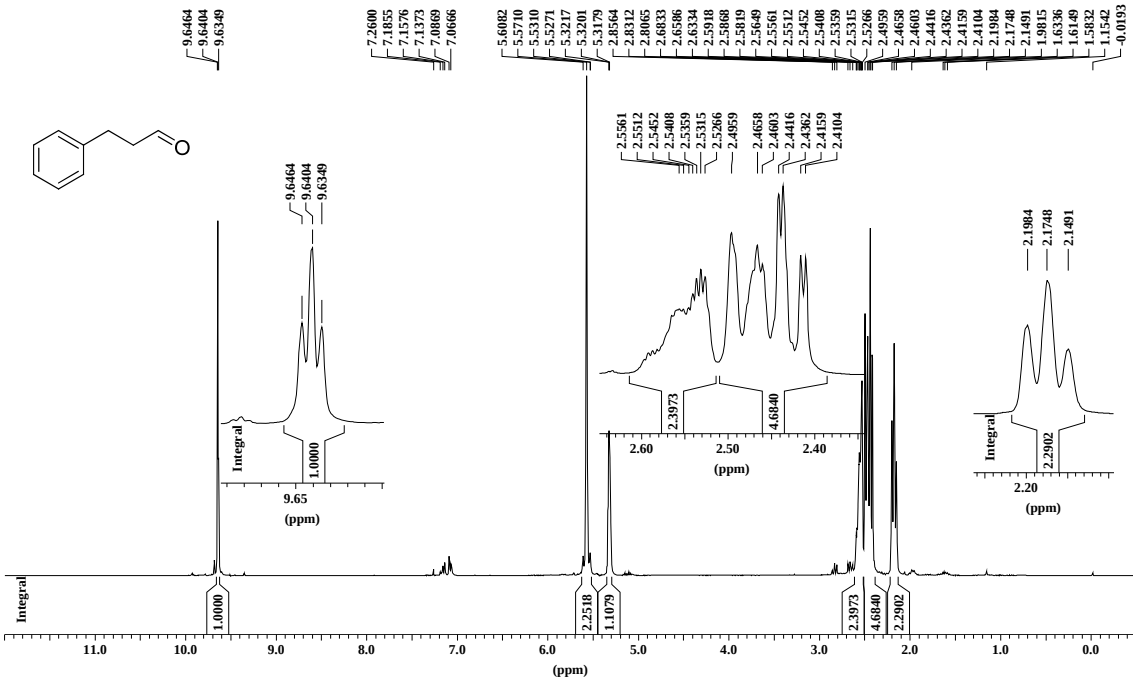


Figure S6. ESI-MS spectra of conjugation reaction of (a) protected **5** with *o*-benzylhydroxylamine; (b) deprotected **5** (treated with 10 mM HCl) with *o*-benzylhydroxylamine

a)



b)

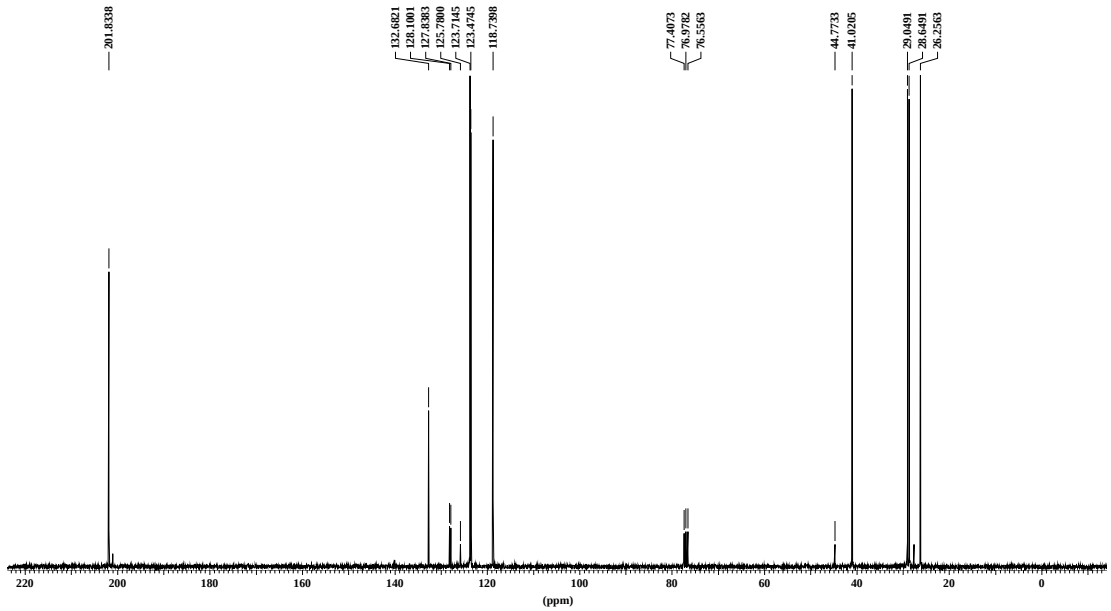
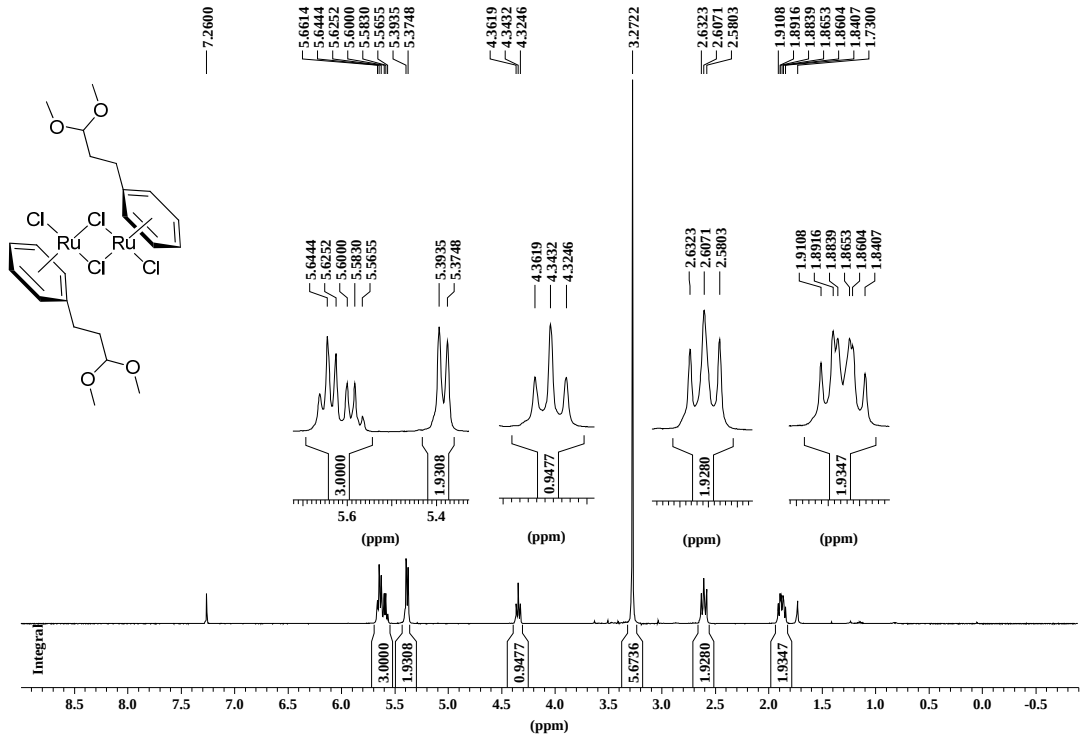


Figure S7. (a) ^{1}H-NMR spectrum of **1** in $CDCl_3$; (b) $^{13}C\{^{1}H\}$-NMR spectrum of **1** in $CDCl_3$.

a)



b)

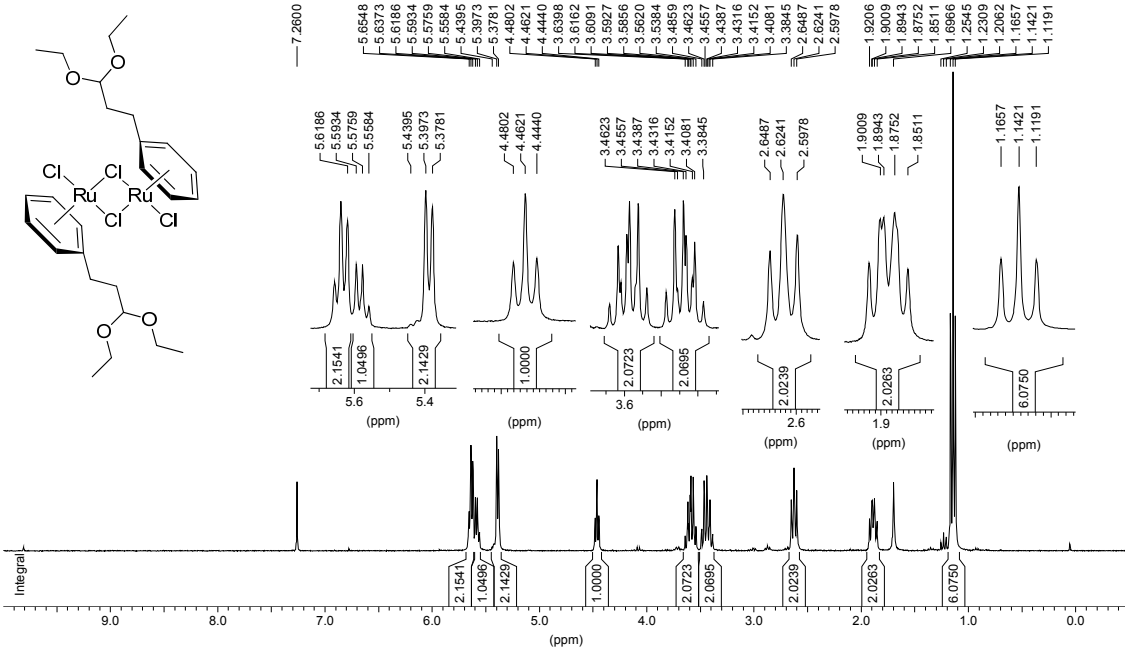
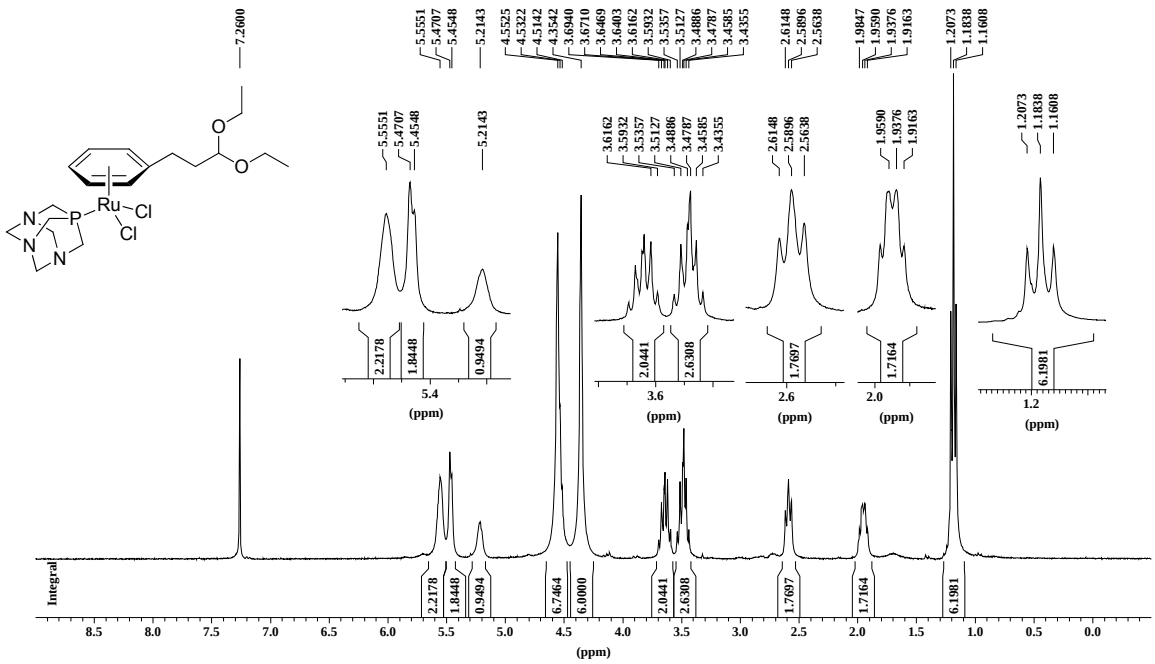


Figure S8. ^{1}H-NMR spectrum of (a) **3a** and (b) **3b** in $CDCl_3$.

a)



b)

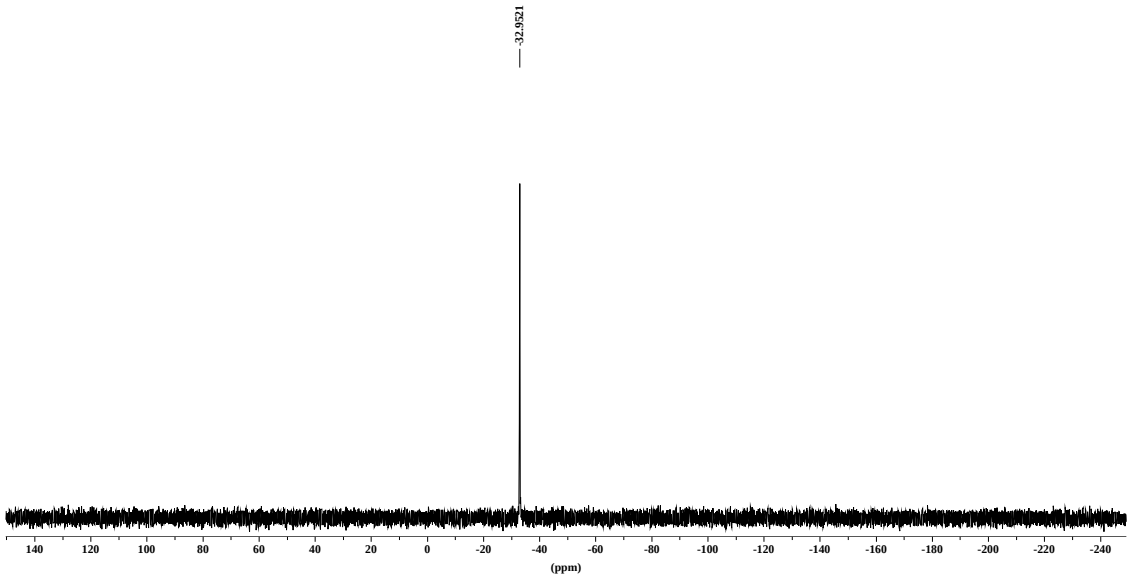
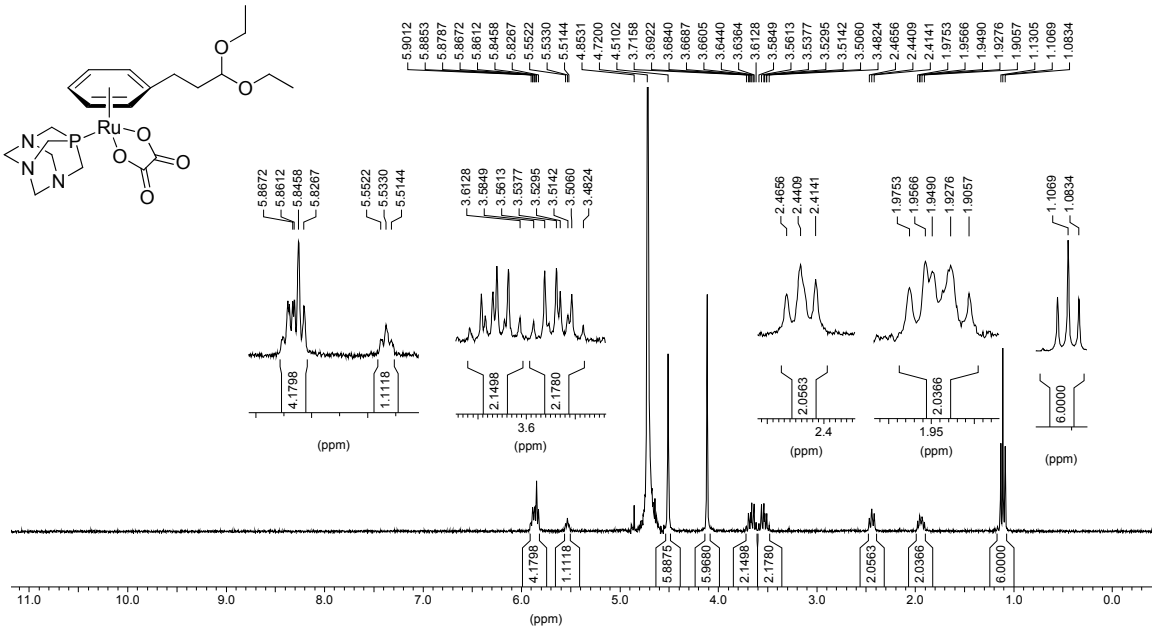


Figure S9. (a) ^{1}H-NMR spectrum of **4** in $CDCl_3$; (b) $^{31}P\{^{1}H\}$-NMR spectrum of **4** in $CDCl_3$.

a)



b)

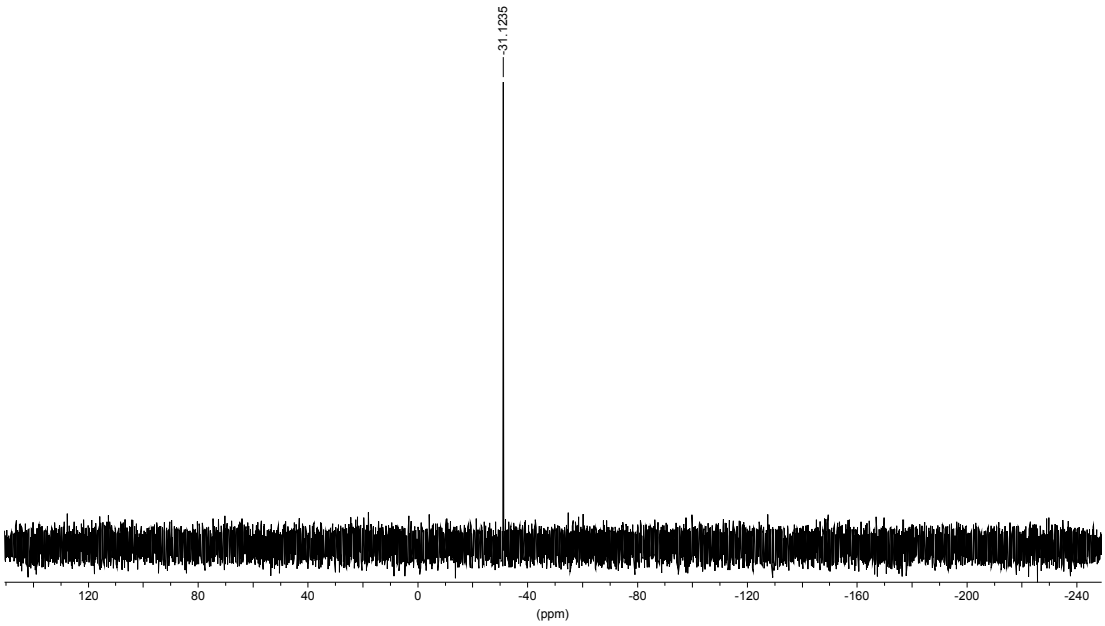


Figure S10. (a) ^{1}H NMR spectrum of **5** in D_2O; (b) $^{31}P\{^{1}H\}$-NMR spectrum of **5** in D_2O.